Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Computational study of aromaticity, ^{1}H NMR spectra and intermolecular interactions of the twisted thia-norhexaphyrin and its multiply annulated polypyrrolic derivatives

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ELECTRONIC SUPPORTING INFORMATION (ESI)

Table S1. ^{1}H chemical shifts (ppm) calculated at the B3LYP/6-311++G** level by the direct comparison with TMS* reference ($\sigma_{TMS} - \sigma_{i(iso)}$) for the porphyrinoids **1**-**5**.

GIAO/B3LYP/ 6-311++G** Gas phase	CSGT/B3LYP/ 6-311++G** Gas phase	GIAO/B3LYP/ 6-311++G** PCM	CSGT/B3LYP/ 6-311++G** PCM	Exp. [17]	Type	Atom num.**	Mol.
8.25	7.30	8.42	7.45	7.87	CH	27	**3**
7.08	6.13	7.28	6.32	7.03	CH	29	
8.96	7.96	9.07	8.05	8.45	CH	98	
8.99	7.92	9.08	7.99	8.53	CH	45	
8.87	7.84	8.98	7.94	8.5	CH	42	
-1.78	-3.24	-1.80	-3.26	0.56	NH	101	
-6.05	-7.22	-6.05	-7.23	-4.41	CH	100	
-6.43	-7.29	-6.34	-7.20	-4.19	NH	99	
8.82	7.80	8.94	7.89	8.38	CH	95	
8.73	7.65	8.86	7.77	8.48	CH	94	
7.46	6.49	7.71	6.72	7.55	CH	96	
7.83	6.83	8.01	7.00	7.57	CH	97	
8.97	7.89	9.07	7.99	8.52	CH	94	**5**
8.94	7.82	9.05	7.92	8.52	CH	95	
-6.64	-7.38	-6.57	-7.31	-4.2	NH	99	
-6.90	-8.11	-6.97	-8.19	-4.96	CH	101	
-5.40	-6.36	-5.43	-6.40	-2.99	NH	100	
9.34	8.26	9.45	8.36	8.88	CH	49	
9.17	8.12	9.27	8.21	8.79	CH	51	
10.04	9.04	10.10	9.08	9.42	CH	98	
8.57	7.54	8.70	7.65	8.33	CH	96	
8.49	7.52	8.65	7.68	8.33	CH	97	
8.06	7.12	8.18	7.23	7.79	CH	34	
7.87	6.86	8.00	6.99	7.76	CH	36	
9.02	8.08	9.20	8.25	8.69	CH	25	**2**
8.02	7.02	8.16	7.15	7.8	CH	27	
8.50	7.48	8.66	7.63	8.25	CH	55	
8.51	7.46	8.63	7.57	8.25	CH	56	
9.24	8.25	9.29	8.27	8.62	CH	68	
-1.22	-2.52	-1.22	-2.52	1.4	NH	72	
8.49	7.46	8.59	7.55	8.14	CH	88	
8.60	7.53	8.70	7.62	8.16	CH	89	
8.37	7.23	8.47	7.32	8.03	CH	17	
7.62	6.47	7.71	6.56	7.37	CH	15	
7.39	6.32	7.77	6.70	8.17	NH	103	**1**
6.59	5.65	6.76	5.82	6.72	CH	104	
6.07	5.10	6.12	5.14	5.93	CH	105	
6.11	5.03	6.24	5.16	6.34	CH	106	
6.23	5.15	6.29	5.21	6.33	CH	35	
10.06	8.72	10.06	8.71	12.06	NH	20	
6.67	5.71	6.77	5.81	6.41	CH	15	
6.61	5.62	6.73	5.73	7.01	CH	17	
9.90	8.62	9.91	8.62	10.59	NH	61	
6.27	5.44	6.31	5.47	6.94	NH	87	
6.53	5.50	6.63	5.58	5.93	CH	68	
6.93	5.80	7.03	5.88	6.27	CH	70	
6.39	5.27	6.53	5.40	6.22	CH	85	
6.41	5.42	6.50	5.51	6.27	CH	84	

5.94	5.07	6.06	5.18	6	CH	45	
6.54	5.63	6.66	5.74	6.41	CH	88	
8.58	7.43	8.57	7.41	8.36	CH	17	**4**
7.20	6.12	7.28	6.20	6.97	CH	15	
7.76	6.67	7.94	6.83	7.76	CH	24	
7.15	6.15	7.34	6.33	7.24	CH	26	
11.03	9.53	11.00	9.49	10.45	CH	43	
5.69	4.47	5.71	4.48	5.33	CH	47	
3.02	2.08	3.07	2.12	3.32	CH	49	
5.64	4.52	5.72	4.59	5.23	CH	50	
6.65	5.63	6.78	5.75	6.5	CH	103	
7.06	6.01	7.15	6.10	6.77	CH	102	
6.45	5.51	6.61	5.66	6.52	CH	87	
6.89	5.87	7.04	6.01	6.87	CH	85	
13.55	11.81	13.53	11.78	13.9	NH	88	

* The TMS reference isotopic shielding constants were taken as 31.9798 ppm (GIAO/B3LYP/6-311++G** gas phase), 30.7300 ppm (CSGT/B3LYP/6-311++G** gas phase), 31.9731 (GIAO/B3LYP/6-311++G** PCM) and 30.7301 (CSGT/B3LYP/6-311++G** PCM).
** Atoms numbering correspond to the Cartesian coordinates presented below in ESI.

Table S2. ^{1}H chemical shifts (ppm) calculated at the B3LYP/6-311++G** level by the linear regression method $\delta_i(\text{theor}) = (\sigma_{TMS} + \sigma_{i(iso)} - b)/a$ for the combined number of H atoms (63 atoms of CH and NH groups) of porphyrinoids **1**-**5***

GIAO/B3LYP/ 6-311++G** Gas phase	CSGT/B3LYP/ 6-311++G** Gas phase	GIAO/B3LYP/ 6-311++G** PCM	CSGT/B3LYP/ 6-311++G** PCM	Exp. [17]	Type	Atom num.**	Mol.
8.12	8.23	8.17	8.28	7.87	CH	27	**3**
7.12	7.22	7.20	7.30	7.03	CH	29	
8.73	8.80	8.73	8.79	8.45	CH	98	
8.76	8.77	8.74	8.74	8.53	CH	45	
8.65	8.70	8.65	8.70	8.5	CH	42	
-0.49	-0.89	-0.55	-0.95	0.56	NH	101	
-4.16	-4.34	-4.19	-4.37	-4.41	CH	100	
-4.48	-4.40	-4.43	-4.35	-4.19	NH	99	
8.61	8.66	8.61	8.66	8.38	CH	95	
8.54	8.54	8.55	8.55	8.48	CH	94	
7.44	7.53	7.57	7.65	7.55	CH	96	
7.76	7.82	7.83	7.89	7.57	CH	97	
8.74	8.75	8.73	8.74	8.52	CH	94	**5**
8.71	8.68	8.72	8.68	8.52	CH	95	
-4.67	-4.47	-4.64	-4.44	-4.2	NH	99	
-4.89	-5.11	-4.97	-5.20	-4.96	CH	101	
-3.60	-3.59	-3.66	-3.66	-2.99	NH	100	
9.06	9.06	9.06	9.06	8.88	CH	49	
8.91	8.94	8.90	8.93	8.79	CH	51	
9.66	9.74	9.61	9.68	9.42	CH	98	
8.40	8.44	8.41	8.45	8.33	CH	96	
8.33	8.42	8.37	8.47	8.33	CH	97	
7.96	8.07	7.97	8.09	7.79	CH	34	
7.79	7.85	7.82	7.88	7.76	CH	36	

8.79	8.91	8.84	8.96	8.69	CH	25	**2**
7.93	7.99	7.95	8.02	7.8	CH	27	
8.34	8.39	8.38	8.43	8.25	CH	55	
8.35	8.37	8.36	8.38	8.25	CH	56	
8.97	9.05	8.91	8.99	8.62	CH	68	
-0.02	-0.27	-0.06	-0.32	1.4	NH	72	
8.33	8.37	8.32	8.36	8.14	CH	88	
8.42	8.43	8.41	8.42	8.16	CH	89	
8.23	8.17	8.22	8.16	8.03	CH	17	
7.58	7.52	7.57	7.51	7.37	CH	15	
7.38	7.38	7.62	7.63	8.17	NH	103	**1**
6.70	6.80	6.76	6.88	6.72	CH	104	
6.25	6.33	6.21	6.28	5.93	CH	105	
6.28	6.26	6.31	6.30	6.34	CH	106	
6.39	6.37	6.36	6.35	6.33	CH	35	
9.67	9.46	9.57	9.36	12.06	NH	20	
6.76	6.86	6.77	6.86	6.41	CH	15	
6.72	6.78	6.73	6.79	7.01	CH	17	
9.54	9.38	9.45	9.28	10.59	NH	61	
6.43	6.62	6.38	6.57	6.94	NH	87	
6.65	6.67	6.64	6.66	5.93	CH	68	
6.99	6.93	6.99	6.93	6.27	CH	70	
6.53	6.47	6.56	6.51	6.22	CH	85	
6.55	6.60	6.54	6.61	6.27	CH	84	
6.13	6.30	6.15	6.32	6	CH	45	
6.65	6.79	6.67	6.80	6.41	CH	88	
8.41	8.34	8.31	8.24	8.36	CH	17	**4**
7.22	7.21	7.20	7.20	6.97	CH	15	
7.71	7.68	7.76	7.75	7.76	CH	24	
7.18	7.24	7.25	7.31	7.24	CH	26	
10.51	10.16	10.38	10.04	10.45	CH	43	
5.92	5.78	5.86	5.72	5.33	CH	47	
3.63	3.71	3.60	3.69	3.32	CH	49	
5.88	5.82	5.87	5.81	5.23	CH	50	
6.74	6.79	6.78	6.81	6.5	CH	103	
7.10	7.12	7.09	7.11	6.77	CH	102	
6.58	6.68	6.63	6.73	6.52	CH	87	
6.96	6.99	7.00	7.03	6.87	CH	85	
12.67	12.13	12.54	12.01	13.9	NH	88	

* The values of parameters *a* and *b* are presented in the Table 1 in the main text.

** Atoms numbering correspond to the Cartesian coordinates presented below in ESI.

Table S3. ^{1}H chemical shifts (ppm) calculated at the B3LYP/6-311++G** level by the linear regression method $\delta_i(\text{theor}) = (\sigma_{TMS} + \sigma_{i(iso)} - b)/a$ for the two separate groups of H atoms (53 and 10 atoms of CH and NH groups, respectively) of porphyrinoids **1**-**5**.*

GIAO/B3LYP/ 6-311++G** Gas phase	CSGT/B3LYP/ 6-311++G** Gas phase	GIAO/B3LYP/ 6-311++G** PCM	CSGT/B3LYP/ 6-311++G** PCM	Exp. [17]	Type	Atom num.**	Mol.
7.95	8.02	7.99	8.06	7.87	CH	27	**3**
6.93	7.02	7.01	7.09	7.03	CH	29	
8.56	8.59	8.55	8.57	8.45	CH	98	
8.59	8.56	8.56	8.53	8.53	CH	45	
8.48	8.49	8.47	8.48	8.50	CH	42	
0.28	-0.11	0.22	-0.18	0.56	NH	101	
-4.47	-4.53	-4.46	-4.52	-4.41	CH	100	
-3.94	-3.88	-3.90	-3.84	-4.19	NH	99	
8.44	8.45	8.44	8.44	8.38	CH	95	
8.37	8.33	8.37	8.33	8.48	CH	94	
7.26	7.32	7.38	7.44	7.55	CH	96	
7.58	7.62	7.64	7.67	7.57	CH	97	
8.57	8.54	8.56	8.52	8.52	CH	94	**5**
8.54	8.47	8.54	8.47	8.52	CH	95	
-4.13	-3.96	-4.11	-3.95	-4.20	NH	99	
-5.20	-5.29	-5.25	-5.35	-4.96	CH	101	
-3.00	-3.01	-3.07	-3.10	-2.99	NH	100	
8.90	8.85	8.88	8.84	8.88	CH	49	
8.74	8.74	8.72	8.71	8.79	CH	51	
9.50	9.53	9.44	9.46	9.42	CH	98	
8.22	8.23	8.23	8.23	8.33	CH	96	
8.15	8.22	8.19	8.25	8.33	CH	97	
7.78	7.87	7.79	7.87	7.79	CH	34	
7.62	7.65	7.63	7.66	7.76	CH	36	
8.62	8.70	8.67	8.74	8.69	CH	25	**2**
7.75	7.78	7.77	7.81	7.80	CH	27	
8.17	8.18	8.20	8.21	8.25	CH	55	
8.17	8.16	8.18	8.16	8.25	CH	56	
8.81	8.84	8.74	8.77	8.62	CH	68	
0.78	0.56	0.74	0.51	1.40	NH	72	
8.16	8.17	8.14	8.14	8.14	CH	88	
8.25	8.22	8.23	8.21	8.16	CH	89	
8.05	7.96	8.04	7.95	8.03	CH	17	
7.40	7.31	7.38	7.30	7.37	CH	15	
8.59	8.79	8.89	9.09	8.17	NH	103	**1**
6.51	6.60	6.57	6.67	6.72	CH	104	
6.05	6.12	6.01	6.08	5.93	CH	105	
6.09	6.06	6.11	6.09	6.34	CH	106	
6.20	6.17	6.16	6.14	6.33	CH	35	
11.02	11.03	10.96	10.96	12.06	NH	20	
6.57	6.65	6.58	6.65	6.41	CH	15	
6.53	6.57	6.54	6.59	7.01	CH	17	
10.88	10.94	10.83	10.88	10.59	NH	61	
7.58	7.97	7.57	7.95	6.94	NH	87	

6.46	6.47	6.45	6.46	5.93	CH	68	
6.80	6.73	6.80	6.72	6.27	CH	70	
6.33	6.27	6.37	6.30	6.22	CH	85	
6.35	6.40	6.34	6.40	6.27	CH	84	
5.94	6.10	5.96	6.11	6.00	CH	45	
6.46	6.58	6.48	6.60	6.41	CH	88	
8.24	8.13	8.12	8.03	8.36	CH	17	**4**
7.04	7.01	7.02	6.99	6.97	CH	15	
7.53	7.48	7.58	7.53	7.76	CH	24	
6.99	7.03	7.06	7.10	7.24	CH	26	
10.36	9.95	10.21	9.81	10.45	CH	43	
5.72	5.58	5.66	5.52	5.33	CH	47	
3.41	3.51	3.39	3.49	3.32	CH	49	
5.68	5.62	5.67	5.60	5.23	CH	50	
6.55	6.58	6.58	6.61	6.50	CH	103	
6.91	6.91	6.90	6.90	6.77	CH	102	
6.38	6.48	6.43	6.52	6.52	CH	87	
6.77	6.79	6.81	6.82	6.87	CH	85	
14.18	13.91	14.11	13.82	13.90	NH	88	

* The values of parameters *a* and *b* are presented in the Table 1 in the main text.

** Atoms numbering correspond to the Cartesian coordinates presented below in ESI.

Table S4. Parameters of the linear correlations $\delta_i(\text{exp}) = (\sigma_{\text{TMS}} - \sigma_{\text{i(iso)}} - b)/a$ for the different groups of protons of the porphyrinoids **1-5** and related values of the mean absolute errors (MAEs) based on the calculations at M06-2X/6-311++G(d,p) level.

	R^2	slope (*a*)	intercept (*b*)	MAE, ppm	MAE(CH), ppm	MAE(NH), ppm
CH+NH (GIAO gas phase)	0.984	1.070	0.040	0.320	0.248	0.699
CH+NH (CSGT gas phase)	0.984	1.056	-0.891	0.320	0.226	0.815
CH+NH (GIAO PCM)	0.983	1.077	0.100	0.338	0.267	0.713
CH+NH (CSGT PCM)	0.983	1.062	-0.850	0.331	0.237	0.825
CH (GIAO gas phase)	0.984	1.033	0.366	–	0.238	–
NH (GIAO gas phase)	0.987	1.079	-0.362	–	–	0.585
CH (CSGT gas phase)	0.988	1.037	-0.666	–	0.211	–
NH (CSGT gas phase)	0.984	1.049	-1.292	–	–	0.676
CH (GIAO PCM)	0.982	1.047	0.395	–	0.259	–
NH (GIAO PCM)	0.987	1.078	-0.323	–	–	0.593
CH (CSGT PCM)	0.988	1.049	-0.655	–	0.218	–
NH (CSGT PCM)	0.983	1.050	-1.263	–	–	0.688
CH+NH (GIAO gas phase) direct	–	–	–	0.634	0.619	0.713
CH+NH (CSGT gas phase) direct	–	–	–	0.600	0.465	1.315
CH+NH (GIAO PCM) direct	–	–	–	0.736	0.737	0.732
CH+NH (CSGT PCM) direct	–	–	–	0.529	0.388	1.277

Table S5. ^{1}H chemical shifts (ppm) calculated at the M06-2X/6-311++G** level by the direct comparison with TMS* reference ($\sigma_{TMS} - \sigma_{i(iso)}$) for the porphyrinoids **1**-**5**.

GIAO/M06-2X/ 6-311++G** Gas phase	CSGT/M06-2X/ 6-311++G** Gas phase	GIAO/M06-2X/ 6-311++G** PCM	CSGT/M06-2X/ 6-311++G** PCM	Exp. [17]	Type	Atom num.**	Mol.
8.06	7.17	8.25	7.34	7.87	CH	27	**3**
7.33	6.40	7.52	6.58	7.03	CH	29	
9.18	8.22	9.29	8.31	8.45	CH	98	
9.30	8.16	9.40	8.24	8.53	CH	45	
9.11	8.07	9.24	8.18	8.50	CH	42	
-0.27	-1.60	-0.41	-1.75	0.56	NH	101	
-4.35	-5.44	-4.47	-5.57	-4.41	CH	100	
-5.10	-5.87	-5.14	-5.92	-4.19	NH	99	
9.45	8.38	9.59	8.50	8.38	CH	95	
9.32	8.25	9.48	8.39	8.48	CH	94	
7.88	6.94	8.13	7.17	7.55	CH	96	
8.26	7.25	9.04	7.41	7.57	CH	97	
8.96	7.99	9.04	8.05	8.52	CH	94	**5**
9.05	7.99	9.15	8.07	8.52	CH	95	
-4.40	-5.12	-4.25	-4.99	-4.20	NH	99	
-4.36	-5.58	-4.34	-5.58	-4.96	CH	101	
-4.01	-4.78	-3.97	-4.76	-2.99	NH	100	
9.81	8.70	9.92	8.79	8.88	CH	49	
9.73	8.56	9.83	8.63	8.79	CH	51	
10.12	9.26	10.15	9.27	9.42	CH	98	
9.23	8.20	9.35	8.30	8.33	CH	96	
8.99	8.01	9.15	8.17	8.33	CH	97	
8.18	7.20	8.30	7.30	7.79	CH	34	
8.43	7.38	8.58	7.51	7.76	CH	36	
9.15	8.15	9.32	8.30	8.69	CH	25	**2**
8.39	7.38	8.54	7.51	7.80	CH	27	
8.85	7.83	9.00	7.98	8.25	CH	55	
8.87	7.91	8.98	8.01	8.25	CH	56	
8.97	8.05	9.01	8.06	8.62	CH	68	
1.30	0.27	1.37	0.33	1.40	NH	72	
8.62	7.55	8.72	7.62	8.14	CH	88	
8.68	7.64	8.78	7.71	8.16	CH	89	
8.32	7.17	8.39	7.24	8.03	CH	17	
7.83	6.70	7.90	6.76	7.37	CH	15	
8.09	6.93	8.49	7.33	8.17	NH	103	**1**
7.23	6.25	7.40	6.42	6.72	CH	104	
6.58	5.54	6.62	5.57	5.93	CH	105	
7.00	5.97	7.09	6.05	6.34	CH	106	
8.07	7.03	8.12	7.08	6.33	CH	35	
12.32	11.04	12.31	11.02	12.06	NH	20	
6.90	6.04	7.00	6.12	6.41	CH	15	
7.08	6.09	7.20	6.19	7.01	CH	17	
13.16	11.93	13.12	11.88	10.59	NH	61	
7.81	6.96	7.84	6.97	6.94	NH	87	
6.72	5.66	6.82	5.75	5.93	CH	68	
7.59	6.42	7.70	6.52	6.27	CH	70	

6.66	5.79	6.82	5.94	6.22	CH	85	
6.75	5.73	6.84	5.81	6.27	CH	84	
6.99	6.10	7.11	6.21	6.00	CH	45	
7.12	6.29	7.24	6.39	6.41	CH	88	
8.87	7.96	8.83	7.91	8.36	CH	17	**4**
7.68	6.66	7.75	6.71	6.97	CH	15	
8.48	7.38	8.66	7.55	7.76	CH	24	
7.84	6.81	8.03	6.99	7.24	CH	26	
10.35	9.24	10.34	9.21	10.45	CH	43	
5.21	4.40	5.23	4.40	5.33	CH	47	
2.60	1.95	2.64	1.98	3.32	CH	49	
5.78	4.87	5.84	4.91	5.23	CH	50	
7.21	6.15	7.34	6.26	6.50	CH	103	
7.68	6.58	7.79	6.67	6.77	CH	102	
7.10	6.07	7.26	6.21	6.52	CH	87	
7.92	6.66	8.07	6.79	6.87	CH	85	
13.60	12.04	13.56	12.00	13.9	NH	88	

* The TMS reference isotopic shielding constants were taken as 32.0753 ppm (GIAO/M06-2X/6-311++G** gas phase), 30.8052 ppm (CSGT/M06-2X/6-311++G** gas phase), 32.0643 (GIAO/M06-2X/6-311++G** PCM) and 30.7945 (CSGT/M06-2X/6-311++G** PCM).
** Atoms numbering correspond to the Cartesian coordinates presented below in ESI.

Table S6. ^{1}H chemical shifts (ppm) calculated at the M06-2X/6-311++G** level by the linear regression method $\delta_i(\text{theor}) = (\sigma_{TMS} + \sigma_{i(iso)} - b)/a$ for the combined number of H atoms (63 atoms of CH and NH groups) of porphyrinoids **1**-**5***

GIAO/M06-2X/ 6-311++G** Gas phase	CSGT/M06-2X/ 6-311++G** Gas phase	GIAO/M06-2X/ 6-311++G** PCM	CSGT/M06-2X/ 6-311++G** PCM	Exp. [17]	Type	Atom num.**	Mol.
7.50	7.64	7.57	7.72	7.87	CH	27	**3**
6.81	6.90	6.89	7.00	7.03	CH	29	
8.54	8.63	8.54	8.63	8.45	CH	98	
8.65	8.57	8.64	8.56	8.53	CH	45	
8.48	8.49	8.49	8.51	8.5	CH	42	
-0.29	-0.67	-0.48	-0.85	0.56	NH	101	
-4.10	-4.31	-4.24	-4.45	-4.41	CH	100	
-4.81	-4.72	-4.87	-4.77	-4.19	NH	99	
8.80	8.78	8.81	8.80	8.38	CH	95	
8.68	8.66	8.71	8.70	8.48	CH	94	
7.33	7.41	7.46	7.56	7.55	CH	96	
7.69	7.71	8.30	7.78	7.57	CH	97	
8.34	8.41	8.30	8.38	8.52	CH	94	**5**
8.43	8.42	8.40	8.40	8.52	CH	95	
-4.15	-4.01	-4.04	-3.90	-4.2	NH	99	
-4.12	-4.44	-4.13	-4.46	-4.96	CH	101	
-3.79	-3.68	-3.78	-3.68	-2.99	NH	100	
9.14	9.08	9.12	9.07	8.88	CH	49	
9.06	8.95	9.03	8.93	8.79	CH	51	
9.42	9.61	9.34	9.53	9.42	CH	98	
8.60	8.61	8.60	8.61	8.33	CH	96	
8.37	8.44	8.41	8.50	8.33	CH	97	

7.61	7.66	7.62	7.68	7.79	CH	34	
7.85	7.83	7.87	7.87	7.76	CH	36	
8.52	8.56	8.56	8.61	8.69	CH	25	**2**
7.81	7.83	7.84	7.87	7.8	CH	27	
8.24	8.26	8.27	8.31	8.25	CH	55	
8.25	8.34	8.25	8.34	8.25	CH	56	
8.35	8.47	8.27	8.39	8.62	CH	68	
1.18	1.10	1.18	1.11	1.4	NH	72	
8.02	7.99	8.01	7.98	8.14	CH	88	
8.08	8.08	8.06	8.06	8.16	CH	89	
7.74	7.64	7.70	7.61	8.03	CH	17	
7.29	7.19	7.25	7.17	7.37	CH	15	
7.53	7.41	7.80	7.70	8.17	NH	103	**1**
6.72	6.76	6.78	6.85	6.72	CH	104	
6.12	6.09	6.06	6.04	5.93	CH	105	
6.51	6.49	6.49	6.50	6.34	CH	106	
7.51	7.51	7.45	7.47	6.33	CH	35	
11.48	11.30	11.34	11.17	12.06	NH	20	
6.41	6.56	6.41	6.57	6.41	CH	15	
6.58	6.61	6.59	6.63	7.01	CH	17	
12.27	12.14	12.10	11.99	10.59	NH	61	
7.27	7.43	7.19	7.37	6.94	NH	87	
6.24	6.21	6.24	6.21	5.93	CH	68	
7.06	6.93	7.06	6.94	6.27	CH	70	
6.19	6.33	6.24	6.39	6.22	CH	85	
6.27	6.27	6.26	6.27	6.27	CH	84	
6.49	6.62	6.51	6.65	6	CH	45	
6.62	6.80	6.63	6.82	6.41	CH	88	
8.26	8.38	8.11	8.25	8.36	CH	17	**4**
7.14	7.15	7.11	7.12	6.97	CH	15	
7.89	7.84	7.95	7.91	7.76	CH	24	
7.29	7.30	7.37	7.39	7.24	CH	26	
9.64	9.59	9.51	9.47	10.45	CH	43	
4.84	5.01	4.77	4.95	5.33	CH	47	
2.39	2.69	2.36	2.66	3.32	CH	49	
5.36	5.46	5.33	5.43	5.23	CH	50	
6.71	6.67	6.73	6.69	6.5	CH	103	
7.14	7.08	7.14	7.08	6.77	CH	102	
6.60	6.59	6.65	6.65	6.52	CH	87	
7.37	7.15	7.40	7.19	6.87	CH	85	
12.68	12.25	12.50	12.10	13.9	NH	88	

* The values of parameters *a* and *b* are presented in the Table S4 in the main text.

** Atoms numbering correspond to the Cartesian coordinates presented below in ESI.

Table S7. ^{1}H chemical shifts (ppm) calculated at the M06-2X/6-311++G** level by the linear regression method $\delta_i(\text{theor}) = (\sigma_{TMS} + \sigma_{i(iso)} - b)/a$ for the two separate groups of H atoms (53 and 10 atoms of CH and NH groups, respectively) of porphyrinoids **1**-**5**.*

GIAO/M06-2X/ 6-311++G** Gas phase	CSGT/M06-2X/ 6-311++G** Gas phase	GIAO/M06-2X/ 6-311++G** PCM	CSGT/M06-2X/ 6-311++G** PCM	Exp. [17]	Type	Atom num.**	Mol.
7.44	7.56	7.51	7.63	7.87	CH	27	**3**
6.73	6.81	6.81	6.90	7.03	CH	29	
8.53	8.57	8.50	8.55	8.45	CH	98	
8.64	8.51	8.60	8.48	8.53	CH	45	
8.46	8.43	8.45	8.43	8.50	CH	42	
0.09	-0.29	-0.08	-0.46	0.56	NH	101	
-4.56	-4.61	-4.65	-4.69	-4.41	CH	100	
-4.40	-4.37	-4.47	-4.44	-4.19	NH	99	
8.79	8.73	8.78	8.73	8.38	CH	95	
8.67	8.61	8.68	8.63	8.48	CH	94	
7.27	7.33	7.39	7.47	7.55	CH	96	
7.64	7.63	8.26	7.70	7.57	CH	97	
8.31	8.35	8.26	8.31	8.52	CH	94	**5**
8.41	8.36	8.36	8.32	8.52	CH	95	
-3.74	-3.66	-3.64	-3.55	-4.20	NH	99	
-4.58	-4.74	-4.53	-4.70	-4.96	CH	101	
-3.38	-3.33	-3.39	-3.33	-2.99	NH	100	
9.14	9.03	9.10	9.00	8.88	CH	49	
9.06	8.90	9.01	8.86	8.79	CH	51	
9.44	9.57	9.32	9.47	9.42	CH	98	
8.58	8.55	8.56	8.54	8.33	CH	96	
8.34	8.37	8.37	8.42	8.33	CH	97	
7.56	7.59	7.55	7.59	7.79	CH	34	
7.81	7.76	7.82	7.78	7.76	CH	36	
8.50	8.50	8.52	8.54	8.69	CH	25	**2**
7.77	7.76	7.78	7.79	7.80	CH	27	
8.21	8.20	8.22	8.23	8.25	CH	55	
8.23	8.28	8.21	8.26	8.25	CH	56	
8.33	8.41	8.23	8.31	8.62	CH	68	
1.54	1.49	1.57	1.52	1.40	NH	72	
7.99	7.92	7.95	7.90	8.14	CH	88	
8.05	8.01	8.01	7.98	8.16	CH	89	
7.69	7.56	7.64	7.53	8.03	CH	17	
7.23	7.11	7.17	7.08	7.37	CH	15	
7.84	7.85	8.18	8.20	8.17	NH	103	**1**
6.64	6.67	6.70	6.75	6.72	CH	104	
6.02	5.99	5.95	5.93	5.93	CH	105	
6.42	6.40	6.40	6.40	6.34	CH	106	
7.45	7.43	7.38	7.38	6.33	CH	35	
11.75	11.76	11.72	11.72	12.06	NH	20	
6.32	6.47	6.31	6.46	6.41	CH	15	
6.49	6.51	6.50	6.53	7.01	CH	17	
12.54	12.61	12.47	12.54	10.59	NH	61	
7.58	7.87	7.57	7.86	6.94	NH	87	

6.15	6.10	6.14	6.10	5.93	CH	68	
6.99	6.84	6.98	6.84	6.27	CH	70	
6.09	6.23	6.14	6.29	6.22	CH	85	
6.18	6.17	6.16	6.17	6.27	CH	84	
6.41	6.53	6.42	6.55	6.00	CH	45	
6.53	6.71	6.54	6.72	6.41	CH	88	
8.23	8.32	8.06	8.17	8.36	CH	17	**4**
7.08	7.06	7.03	7.03	6.97	CH	15	
7.85	7.77	7.90	7.82	7.76	CH	24	
7.23	7.22	7.30	7.29	7.24	CH	26	
9.66	9.55	9.50	9.41	10.45	CH	43	
4.69	4.88	4.62	4.82	5.33	CH	47	
2.16	2.52	2.15	2.51	3.32	CH	49	
5.24	5.34	5.20	5.31	5.23	CH	50	
6.62	6.57	6.64	6.59	6.50	CH	103	
7.08	6.99	7.06	6.99	6.77	CH	102	
6.51	6.50	6.56	6.54	6.52	CH	87	
7.31	7.07	7.33	7.10	6.87	CH	85	
12.95	12.72	12.88	12.65	13.90	NH	88	

* The values of parameters *a* and *b* are presented in the Table S4 in the main text.

** Atoms numbering correspond to the Cartesian coordinates presented below in ESI.

Table S8. Topological characteristics* of the non-covalent interactions calculated by the QTAIM method for the porphyrinoids **1-5**.

Bond	*d*. Å	$\rho(\mathbf{r})$. $e \cdot a_o^{-3}$ *	$v(\mathbf{r})$. a.u.	$g(\mathbf{r})$. a.u.	$h_e(\mathbf{r})$. a.u.	$\nabla^2\rho(\mathbf{r})$. $e \cdot a_o^{-5}$	E kcal mol^{-1}	ε
1 (geometry from B3LYP/6-31G(d) optimization)								
N1H---N2	**2.083**	**0.0241**	**-0.0185**	**0.0188**	**0.0003**	**0.0763**	**-5.8**	**0.029**
N3H---N2	**2.058**	**0.0254**	**-0.0196**	**0.0198**	**0.0002**	**0.0804**	**-6.1**	**0.034**
N4H---C3	2.522	0.0106	-0.0067	0.0084	0.0017	0.0410	-2.1	0.923
C1H---N1	2.637	0.0099	-0.0059	0.0083	0.0024	0.0431	-1.9	0.170
C2H---F4	3.573	0.0004	-0.0002	0.0004	0.0002	0.0025	-0.1	0.224
N3---C1	3.950	0.0018	-0.0010	0.0013	0.0003	0.0069	-0.3	1.214
F3---C4	3.421	0.0030	-0.0018	0.0027	0.0009	0.0144	-0.6	0.332
F1---F2	2.867	0.0052	-0.0055	0.0069	0.0014	0.0328	-1.7	0.051
F1---F3	2.695	0.0098	-0.0102	0.0112	0.0010	0.0487	-3.2	0.054
1 (geometry from single crystal X-ray analysis)								
N1H---N2	**2.116**	**0.0227**	**-0.0183**	**0.0200**	**0.0017**	**0.0873**	**-5.7**	**0.062**
N3H---N2	**2.227**	**0.0181**	**-0.0138**	**0.0159**	**0.0021**	**0.0720**	**-4.3**	**0.185**
N4---C3	3.039	0.0101	-0.0060	0.0073	0.0013	0.0350	-1.9	3.071
N4---S	3.280	0.0101	-0.0060	0.0070	0.0010	0.0315	-1.9	1.707
C1H---HN1	1.989	0.0105	-0.0073	0.0103	0.0030	0.0534	-2.3	0.224
C2H---F4	3.492	0.0005	-0.0002	0.0005	0.0003	0.0033	-0.1	0.163
N3---C1	3.667	0.0032	-0.0017	0.0021	0.0004	0.0102	-0.5	0.529
F3---C4	3.580	0.0019	-0.0011	0.0019	0.0008	0.0108	-0.3	2.370
F1---F3	2.673	0.0092	-0.0098	0.0107	0.0009	0.0466	-3.1	0.048
2 (geometry from B3LYP/6-31G(d) optimization)								
N2H---S	**2.360**	**0.0199**	**-0.0157**	**0.0165**	**0.0008**	**0.0697**	**-4.9**	**0.193**
N2H---N3	**2.068**	**0.0246**	**-0.0193**	**0.0197**	**0.0004**	**0.0807**	**-6.1**	**0.063**
N3---S	**3.027**	**0.0166**	**-0.0105**	**0.0114**	**0.0009**	**0.0495**	**-3.3**	**0.063**
N5---C5	3.271	0.0065	-0.0040	0.0047	0.0007	0.0224	-1.3	2.628
F5---C6	2.942	0.0091	-0.0067	0.0081	0.0014	0.0379	-2.1	0.465
F6---C7	2.962	0.0085	-0.0063	0.0079	0.0016	0.0384	-2.0	1.864
2 (geometry from single crystal X-ray analysis)								
N2H---S	**2.455**	**0.0165**	**-0.0130**	**0.0157**	**0.0027**	**0.0736**	**-4.1**	**0.275**
N2H---N3	**2.142**	**0.0202**	**-0.0169**	**0.0189**	**0.0020**	**0.0839**	**-5.3**	**0.063**
N3---S	**2.991**	**0.0175**	**-0.0112**	**0.0122**	**0.0010**	**0.0529**	**-3.5**	**0.046**
F5---C6	2.900	0.0100	-0.0076	0.0088	0.0012	0.0406	-2.4	0.184
F6---C7	2.928	0.0091	-0.0067	0.0085	0.0018	0.0408	-2.1	2.281
4 (geometry from B3LYP/6-31G(d) optimization)								
N1H---N2	**1.946**	**0.0315**	**-0.0253**	**0.0251**	**-0.0002**	**0.0996**	**-7.9**	**0.025**
N1H---S	**2.751**	**0.0106**	**-0.0062**	**0.0080**	**0.0018**	**0.0391**	**-1.9**	**0.430**
N2---HC8	**2.508**	**0.0115**	**-0.0072**	**0.0084**	**0.0012**	**0.0386**	**-2.3**	**0.131**
C8H---F7	2.502	0.0073	-0.0054	0.0068	0.0014	0.0327	-1.7	0.068
O---HC13	**2.225**	**0.0191**	**-0.0155**	**0.0172**	**0.0017**	**0.0754**	**-4.9**	**0.709**
O---C9	3.325	0.0052	-0.0031	0.0039	0.0008	0.0186	-1.0	2.134
N5---HC6	**2.126**	**0.0227**	**-0.0166**	**0.0175**	**0.0009**	**0.0735**	**-5.2**	**0.051**
C12---F5	2.977	0.0082	-0.0059	0.0075	0.0016	0.0363	-1.9	2.370
C11---F12	3.080	0.0067	-0.0047	0.0063	0.0016	0.0321	-1.5	0.745
C10---F11	2.904	0.0094	-0.0071	0.0087	0.0016	0.0420	-2.2	0.733
F7---F8	2.833	0.0064	-0.0067	0.0080	0.0013	0.0376	-2.1	0.044
F8---F9	2.862	0.0066	-0.0068	0.0083	0.0015	0.0386	-2.1	0.100
F9---F10	2.851	0.0060	-0.0063	0.0076	0.0013	0.0359	-2.0	0.061
4 (geometry from single crystal X-ray analysis)								
N1H---N2	2.018	**0.0272**	**-0.0234**	**0.0258**	**0.0023**	**0.1127**	**-7.3**	**0.068**
N1H---S	**2.571**	**0.0145**	**-0.0102**	**0.0126**	**0.0024**	**0.0603**	**-3.2**	**0.351**
N2---HC8	**2.604**	**0.0092**	**-0.0056**	**0.0071**	**0.0015**	**0.0343**	**-1.8**	**0.298**
O---HC13	**2.227**	**0.0188**	**-0.0156**	**0.0178**	**0.0022**	**0.0800**	**-4.9**	**1.044**
O---C9	3.189	0.0068	-0.0040	0.0050	0.0010	0.0238	-1.3	1.698
N5---HC6	**2.242**	**0.0182**	**-0.0130**	**0.0149**	**0.0019**	**0.0674**	**-4.1**	**0.111**

C12---F5	2.937	0.0086	-0.0063	0.0080	0.0017	0.0388	-2.0	2.016
C11---F12	3.059	0.0065	-0.0045	0.0061	0.0016	0.0310	-1.4	2.758
C10---F11	2.917	0.0091	-0.0069	0.0090	0.0021	0.0446	-2.2	1.186
F8---F9	2.905	0.0061	-0.0058	0.0074	0.0016	0.0361	-1.8	3.837
F9---F10	2.964	0.0045	-0.0046	0.0061	0.0015	0.0303	-1.4	0.038
3 (geometry from B3LYP/6-31G(d) optimization)								
N3---HN2	**1.909**	**0.0348**	**-0.0283**	**0.0278**	**-0.0005**	**0.1094**	**-8.9**	**0.056**
N2H---N1	2.562	0.0095	-0.0065	0.0086	0.0021	0.0430	-2.0	0.317
N1---HC13	**2.288**	**0.0167**	**-0.0118**	**0.0145**	**0.0027**	**0.0689**	**-3.7**	**0.457**
C14---H	2.470	0.0129	-0.0076	0.0094	0.0018	0.0451	-2.4	0.286
3 (geometry from single crystal X-ray analysis)								
N3---HN2	**1.822**	**0.0403**	**-0.0383**	**0.0398**	**0.0015**	**0.1653**	**-12.0**	**0.024**
N2---N1	3.061	0.0070	-0.0047	0.0066	0.0019	0.0335	-1.5	1.084
N1---HC13	**2.261**	**0.0168**	**-0.0129**	**0.0167**	**0.0038**	**0.0823**	**-4.0**	**0.623**
C14---H	2.592	0.0108	-0.0060	0.0083	0.0023	0.0418	-1.9	0.249
F8---C15	2.982	0.0084	-0.0061	0.0077	0.0016	0.0370	-1.9	1.996
F7---F8	3.332	0.0013	-0.0012	0.0022	0.0010	0.0131	-0.4	1.926
5 (geometry from B3LYP/6-31G(d) optimization)								
N1---HN2	**2.352**	**0.0149**	**-0.0109**	**0.0139**	**0.0030**	**0.0676**	**-3.4**	**0.769**
N2H---N3	**2.268**	**0.0166**	**-0.0120**	**0.0130**	**0.0010**	**0.0561**	**-3.8**	**0.143**
N3---HC16	**2.234**	**0.0185**	**-0.0129**	**0.0135**	**0.0006**	**0.0571**	**-4.0**	**0.024**
C16H---N1	2.315	0.0165	-0.0120	0.0157	0.0037	0.0779	-3.8	1.792
C14---H	2.747	0.0080	-0.0039	0.0055	0.0015	0.0282	-1.2	2.124
C7---F6	2.956	0.0086	-0.0063	0.0080	0.0017	0.0390	-2.0	1.750
5 (geometry from single crystal X-ray analysis)								
N1---HN2	**2.358**	**0.0122**	**-0.0092**	**0.0128**	**0.0036**	**0.0662**	**-2.9**	**0.508**
N2H---N3	**2.481**	**0.0114**	**-0.0079**	**0.0101**	**0.0022**	**0.0493**	**-2.5**	**0.508**
N3---HC16	**2.388**	**0.0134**	**-0.0089**	**0.0102**	**0.0013**	**0.0464**	**-2.8**	**0.056**
C14---H	2.708	0.0084	-0.0044	0.0061	-0.0016	0.0313	-1.4	1.015
C7H---F6	2.474	0.0090	-0.0069	0.0091	-0.0022	0.0455	-2.2	0.641

* d – interatomic distance, $\rho(\mathbf{r})$ – electron density in bond critical point (BCP), $v(\mathbf{r})$ – potential energy density in BCP, $g(\mathbf{r})$ – kinetic energy density in BCP, $h_e(\mathbf{r})$ – electronic energy density in BCP ($v(\mathbf{r})+g(\mathbf{r})$), $\nabla^2\rho(\mathbf{r})$ – Laplacian of electron density in BCP, E – EML bond energy, ε – bond elipticity; a_0 – Bohr radius.

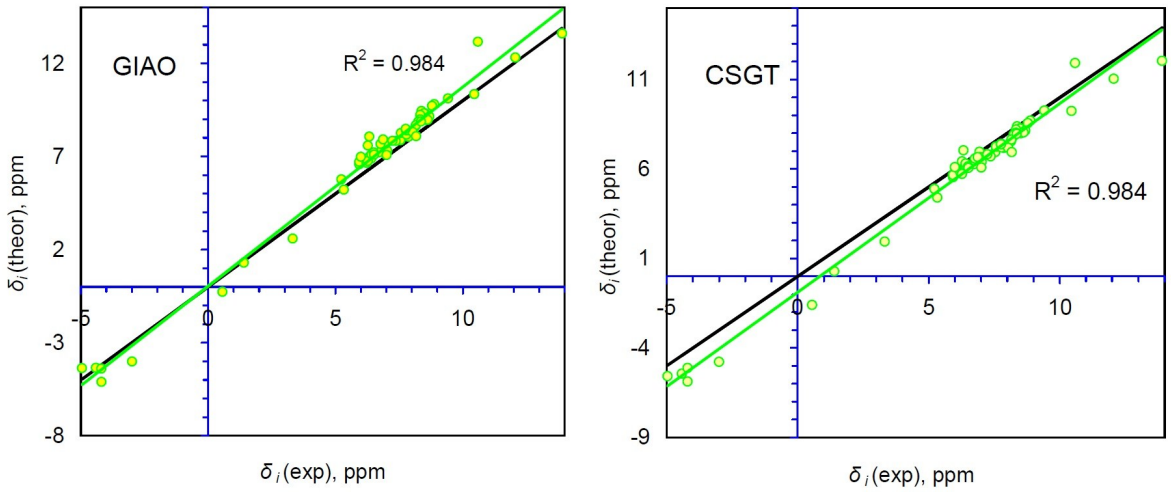

Figure S1. Comparison between the M06-2X/6-311++G(d,p) calculated and experimentally determined ^{1}H chemical shifts for the single group of protons containing 63 atoms of NH and CH types. R^2 parameter corresponds to the linear correlation (green line) between the δ_i(exp) and δ_i(theor). Idealized correlation δ_i(theor)=δ_i(exp) (black line) is presented for comparison. Experimental data are taken from Ref. [17].

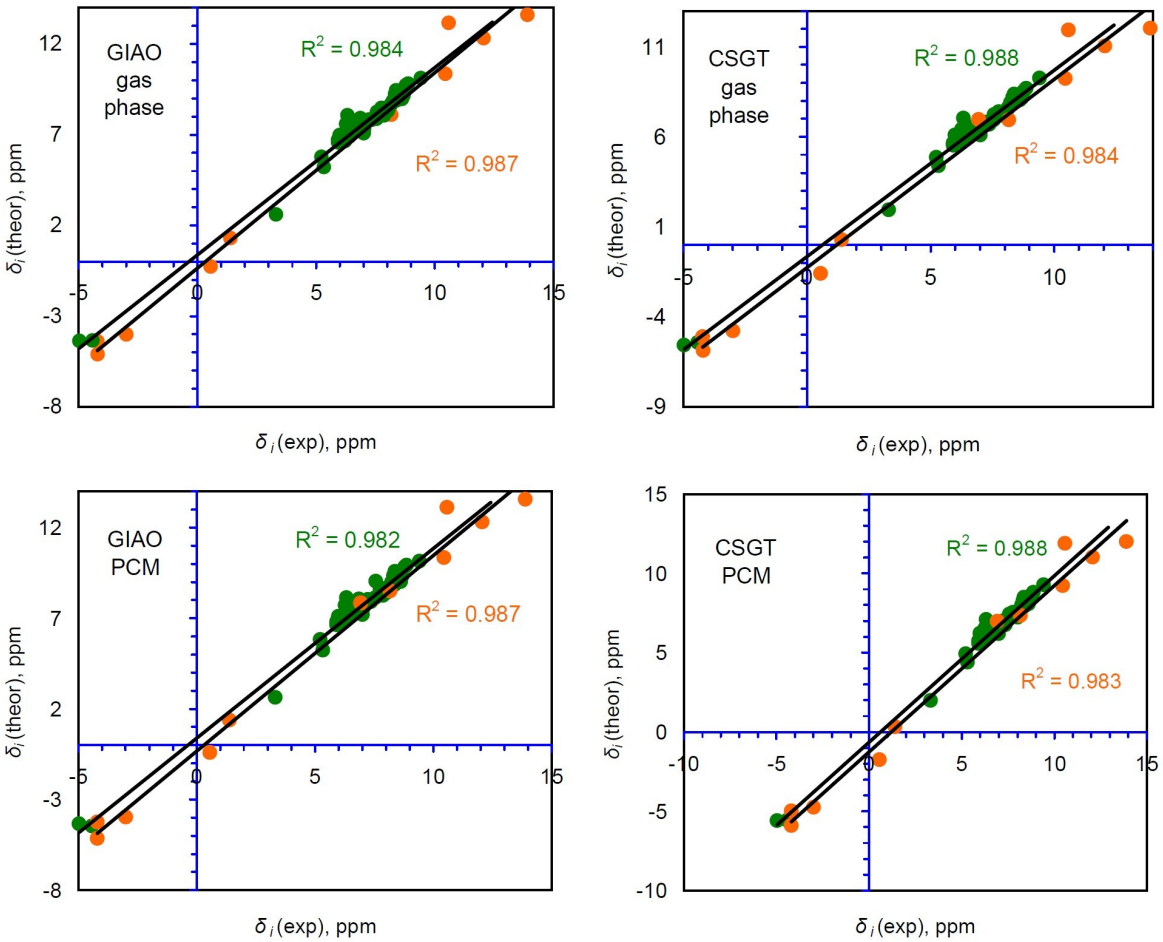

Figure S2. Comparison between the M06-2X/6-311++G(d,p) calculated and experimentally found ^{1}H chemical shifts for the two groups of CH (52 atoms, green spots) and NH (11 atoms, orange spots) types, calculated both by the GIAO and CSGT schemes with and without accounting of solvent effect at the PCM level. R^2 parameter corresponds to the linear correlation (black line) between the δ_i(exp) and δ_i(theor).

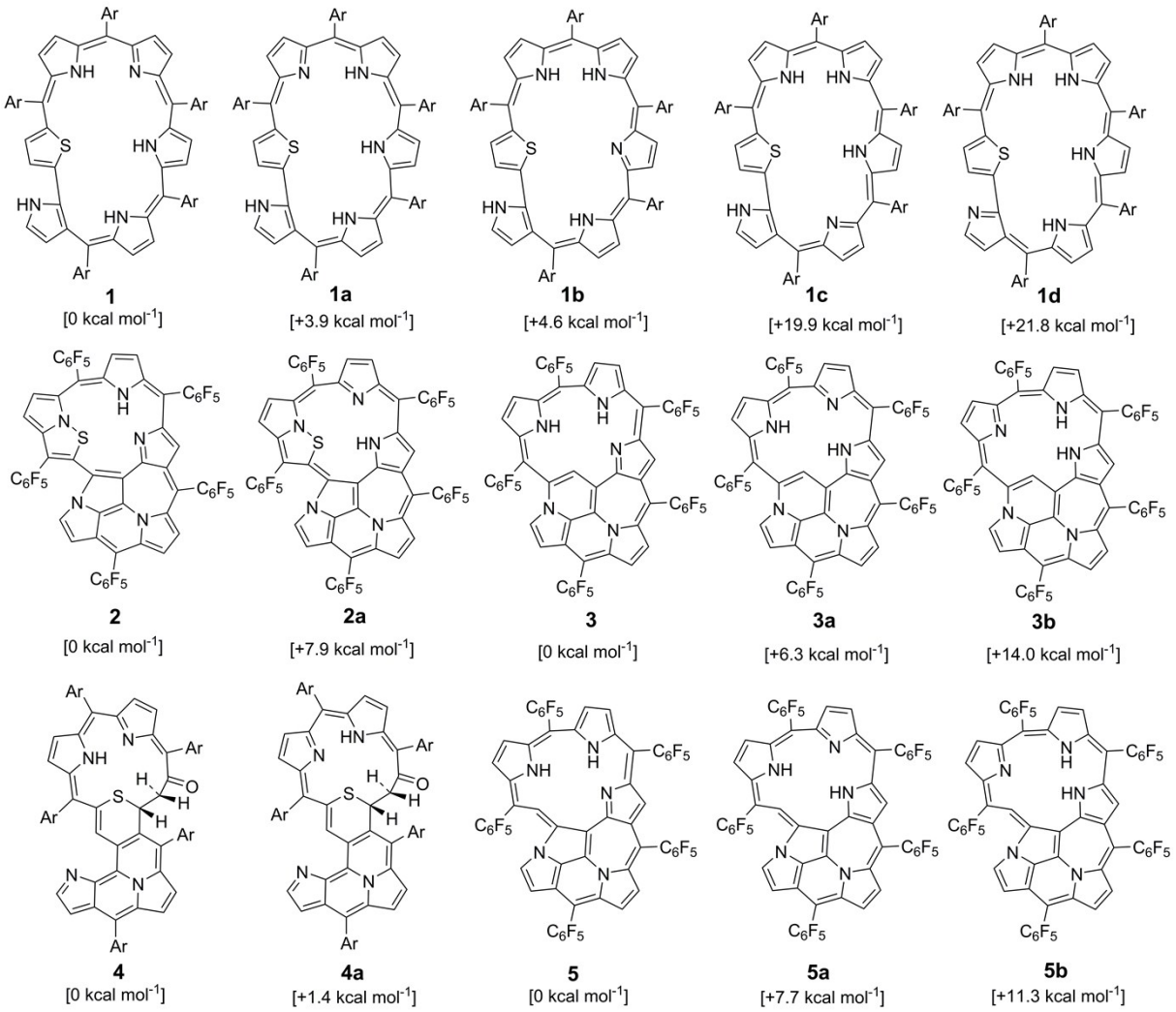

Figure S3. The possible tautomers of porphyrinoids **1**-**5** and their energies relative to the most stable form (taken as 0 kcal mol^{-1}) calculated by the B3LYP/6-31G(d) method.

Table S9. Atomic Cartesian coordinates for the porphyrinoid **1** optimized by the B3LYP/6-31G(d) method. First column contains atomic numbers.

1	9	-9.078106669	-4.590730329	-0.473010034
2	6	-7.940276575	-3.892742278	-0.510390037
3	6	-7.583285559	-3.078094224	0.561538041
4	9	-8.379409605	-3.000813215	1.633810118
5	6	-6.391520450	-2.360535171	0.512922037
6	9	-6.077729454	-1.600670117	1.570727115
7	6	-5.523545405	-2.418947174	-0.587668041
8	6	-5.922831441	-3.240263232	-1.651517119
9	6	-7.104288495	-3.976824289	-1.620698116
10	9	-7.448906553	-4.748874342	-2.658256192
11	9	-5.163050373	-3.334495238	-2.753530200
12	6	-4.272755309	-1.617732115	-0.617169043
13	6	-3.055892222	-2.265086164	-0.794478056
14	6	-2.775995198	-3.678621267	-0.912029067
15	1	-3.517420256	-4.460169321	-0.832278060
16	6	-1.444278105	-3.836704276	-1.139247083
17	1	-0.921961068	-4.767845341	-1.303571092
18	6	-0.817382059	-2.530774180	-1.182741087
19	7	-1.841701131	-1.625165118	-0.955547069
20	1	-1.774499129	-0.620703042	-0.825500062
21	6	0.514406037	-2.239386163	-1.434080103
22	6	1.485537108	-3.365286242	-1.477020106
23	6	1.664932122	-4.251227304	-0.402276029
24	9	0.934805067	-4.124780295	0.713383050
25	6	2.592291189	-5.289633381	-0.442895032
26	9	2.735052199	-6.109324458	0.604850045
27	6	3.380850244	-5.469482381	-1.575807116
28	9	4.272875305	-6.461332476	-1.621763117
29	6	3.230684235	-4.612303330	-2.663402192
30	6	2.291452166	-3.588028260	-2.606222188
31	9	2.162300156	-2.804364200	-3.685012267
32	9	3.973066283	-4.791629345	-3.761308271
33	6	1.011309074	-0.900929066	-1.675712119
34	6	0.347657025	0.222791016	-2.151461156
35	1	-0.692843051	0.216735016	-2.453003175
36	6	1.165644085	1.367981097	-2.258729163
37	6	2.481188177	1.158200085	-1.875489135
38	16	2.704877194	-0.505576036	-1.377781099
39	6	3.557429257	2.127847150	-1.891484137
40	6	4.698795341	2.326125167	-1.087885081
41	6	5.087193365	1.621163115	0.137219010
42	6	4.194529301	1.319546096	1.142067084
43	6	4.340851314	0.426794031	2.275167165
44	6	3.121147222	0.248102018	2.850747205
45	1	2.888874209	-0.369679027	3.706807269
46	6	2.149599156	1.047918075	2.134862152
47	6	0.772282055	1.105178080	2.266678162
48	6	0.055664004	0.071152005	3.045805220
49	6	0.257405018	-1.301059093	2.822424204
50	6	-0.432801031	-2.281389162	3.529711255
51	9	-0.212348015	-3.577332259	3.283852234
52	6	-1.374246100	-1.905326138	4.484657321
53	9	-2.045137149	-2.835860205	5.167238372
54	6	-1.612964117	-0.553515042	4.726015340
55	9	-2.508315178	-0.190906014	5.650712413
56	6	-0.902664064	0.408910030	4.015851291
57	9	-1.148945082	1.697129123	4.287990306
58	9	1.130352079	-1.707597122	1.888283138
59	6	0.005227000	2.105978149	1.562704110

60	7	-1.246101088	1.877324137	1.062381076
61	1	-1.744918126	0.992706070	0.995196071
62	6	-1.757779128	3.013955216	0.468390033
63	6	-3.036431221	3.052830217	-0.148585011
64	6	-3.817047272	1.921993137	-0.390270028
65	7	-3.342330242	0.625392045	-0.250019018
66	6	-4.381145314	-0.186738013	-0.522585038
67	6	-5.577530427	0.583278040	-0.823695059
68	1	-6.546137469	0.176766013	-1.082129077
69	6	-5.213347374	1.895048135	-0.780154054
70	1	-5.839853432	2.756419196	-0.967710071
71	6	-3.551412258	4.396358319	-0.549566041
72	6	-4.568510330	5.042337364	0.159958011
73	9	-5.117398368	4.453870318	1.230375088
74	6	-5.048125362	6.295962469	-0.213944015
75	9	-6.024771458	6.884474510	0.484512035
76	6	-4.498841325	6.941555484	-1.318901097
77	6	-3.479604249	6.327872439	-2.043066145
78	6	-3.023193217	5.071162363	-1.654721118
79	9	-2.041282145	4.508189326	-2.377366172
80	9	-2.950457211	6.944005522	-3.106642225
81	9	-4.947821354	8.144777599	-1.683646121
82	6	-0.780785055	4.022209292	0.629637046
83	6	0.311102022	3.460522250	1.285888094
84	1	1.207450087	3.971267287	1.609350117
85	1	-0.883406065	5.049681365	0.310437022
86	7	2.871496208	1.740430126	1.180276084
87	1	2.425218173	2.219187160	0.411492029
88	1	5.269258379	-0.043585003	2.565919186
89	6	6.514190456	1.253941092	0.285705020
90	6	7.183101509	0.535855037	-0.719974053
91	9	6.510836478	0.116143008	-1.800757131
92	6	8.532378608	0.210130015	-0.632142045
93	9	9.127632633	-0.486257035	-1.607249114
94	6	9.263126668	0.594718042	0.490298035
95	6	8.634826636	1.302755095	1.511136110
96	6	7.285239544	1.626549118	1.397893100
97	9	6.733950465	2.333144168	2.397324172
98	9	9.334426688	1.684412121	2.586540186
99	9	10.557628736	0.281445020	0.588132045
100	6	5.437362381	3.399482247	-1.681685122
101	6	4.739801338	3.841535278	-2.778725202
102	7	3.602288258	3.082674221	-2.890251207
103	1	2.972244216	3.088797220	-3.678635264
104	1	4.950972356	4.636428336	-3.479272249
105	1	6.359273446	3.817187277	-1.301833094
106	1	0.788565056	2.335184168	-2.576555183

Table S10. Atomic Cartesian coordinates for the porphyrinoid **2** optimized by the B3LYP/6-31G(d) method. First column contains atomic numbers.

1	9	2.294711168	-7.036868509	3.443209248
2	6	1.572645113	-6.221939462	2.671454190
3	6	0.801816056	-6.740613495	1.634133117
4	9	0.787067056	-8.058408569	1.406191102
5	6	0.057832004	-5.878881418	0.833173058
6	9	-0.664728049	-6.417510461	-0.161489012
7	6	0.048870004	-4.490357322	1.029615072
8	6	0.822235059	-4.005845290	2.094336149
9	6	1.585267112	-4.848076348	2.898761208
10	9	2.311958166	-4.345935315	3.902055279
11	9	0.842351060	-2.696464192	2.373303170
12	6	-0.782860054	-3.610477260	0.180740013
13	6	-2.190148156	-3.797157272	0.083634006
14	6	-3.213017229	-4.630443336	0.571566040
15	1	-3.072699219	-5.551326416	1.118936080
16	6	-4.424508321	-4.009380289	0.275497020
17	1	-5.405317364	-4.346692314	0.581711040
18	6	-4.185369301	-2.763058201	-0.366391027
19	7	-2.812258202	-2.710333197	-0.520315038
20	16	-1.697179120	-1.717838126	-1.370946098
21	6	-0.367975027	-2.424355175	-0.434176031
22	6	0.877340064	-1.733577127	-0.406593029
23	7	2.118885153	-2.436323175	-0.452843032
24	6	2.760048198	-3.618113262	-0.847222063
25	1	2.201885160	-4.520698324	-1.045759074
26	6	4.129351296	-3.404001246	-0.899965064
27	1	4.857171349	-4.165434300	-1.143200085
28	6	4.380654317	-2.015959146	-0.570836040
29	6	5.377766386	-1.011053074	-0.555127038
30	6	6.802786477	-1.319085098	-0.814399061
31	6	7.448730549	-2.357156168	-0.125813009
32	9	6.786568464	-3.056495219	0.806787058
33	6	8.776719641	-2.696039193	-0.365967027
34	9	9.356898676	-3.685270268	0.319974023
35	6	9.504798690	-1.992636146	-1.322807097
36	9	10.778566799	-2.307201164	-1.560172114
37	6	8.894897621	-0.960737070	-2.031681145
38	6	7.562714534	-0.643553048	-1.780570130
39	9	7.011092497	0.334737024	-2.512348181
40	9	9.583246677	-0.293176021	-2.962560214
41	6	4.959607359	0.323055023	-0.296838021
42	7	3.592106258	0.690177051	-0.152995011
43	6	2.620949190	-0.261740019	-0.188111014
44	6	3.105186226	-1.531541111	-0.300250022
45	6	1.189546084	-0.337132024	-0.220660016
46	6	0.386744028	0.840427062	-0.007420001
47	7	-0.931590067	0.853204062	0.031892002
48	6	-1.344429095	2.183598159	0.166123012
49	6	-0.228586016	3.023775216	0.282522020
50	6	0.927259069	2.225715159	0.163782012
51	6	2.248124160	2.737292195	0.192393014
52	6	3.466982250	2.065186151	0.041452003
53	6	4.803552348	2.573257186	0.046543003
54	6	5.687650413	1.541096110	-0.153347011
55	1	6.763691497	1.619429117	-0.197630014
56	1	5.057213362	3.613474261	0.189106014
57	6	2.385111173	4.217548305	0.397424028
58	6	2.246377160	4.790911346	1.664497122
59	9	1.998557142	4.014068291	2.726140198

60	6	2.359975169	6.164477427	1.865470132
61	9	2.226095162	6.684789475	3.089568221
62	6	2.620834190	6.998495486	0.780138056
63	6	2.766155200	6.455545446	-0.494442035
64	6	2.646573191	5.078819367	-0.671444049
65	9	2.794002200	4.584686331	-1.907520139
66	9	3.018894218	7.254367502	-1.535867109
67	9	2.734660195	8.315358573	0.962360068
68	1	-0.247359018	4.096595293	0.397953028
69	6	-2.718219197	2.556013183	0.083518006
70	6	-3.767982270	1.657649119	-0.139216010
71	7	-3.654165261	0.283563020	-0.143043010
72	1	-2.746735199	-0.137444010	0.031914002
73	6	-4.847981350	-0.326934024	-0.496302036
74	6	-5.117384366	-1.696261124	-0.576906042
75	6	-6.528613447	-2.124785151	-0.780614057
76	6	-6.885085498	-2.915552209	-1.883383137
77	9	-5.959909409	-3.252785233	-2.791450201
78	6	-8.187554594	-3.359903244	-2.090162153
79	9	-8.490546617	-4.102356298	-3.161197230
80	6	-9.184171676	-3.016772217	-1.179288084
81	6	-8.867684628	-2.235560164	-0.071017005
82	6	-7.555576568	-1.808516129	0.120251009
83	9	-7.293945516	-1.082165077	1.215476087
84	9	-9.820092708	-1.915550139	0.812819059
85	9	-10.438157764	-3.434313249	-1.369232098
86	6	-5.776909439	0.757412053	-0.711541053
87	6	-5.138307368	1.941814137	-0.478935034
88	1	-5.556791389	2.933687214	-0.572118041
89	1	-6.804078516	0.628107047	-1.020529072
90	6	-3.066585222	4.002074288	0.173195012
91	6	-3.830094275	4.502589323	1.236199091
92	9	-4.259568307	3.677221265	2.200220156
93	6	-4.167963301	5.849910446	1.340261099
94	9	-4.896755353	6.289743472	2.372809173
95	6	-3.733993268	6.745013498	0.366062027
96	6	-2.971530213	6.283842457	-0.704162052
97	6	-2.655718189	4.930324357	-0.792427055
98	9	-1.936719139	4.527655328	-1.849882132
99	9	-2.560912185	7.139714531	-1.648217117
100	9	-4.048228291	8.040137561	0.456527033

Table S11. Atomic Cartesian coordinates for the porphyrinoid **3** optimized by the B3LYP/6-31G(d) method. First column contains atomic numbers.

1	9	-7.974241552	-4.617656334	-2.747382198
2	6	-7.710257565	-3.822902275	-1.703858125
3	6	-6.450687440	-3.248335233	-1.553476111
4	9	-5.527575407	-3.517772254	-2.486188177
5	6	-6.137607447	-2.406498174	-0.477962034
6	6	-4.780136345	-1.804520132	-0.332270024
7	6	-3.728312270	-2.707227196	-0.086831006
8	6	-3.831087276	-4.064660293	0.333444024
9	6	-2.566595183	-4.558062329	0.556049039
10	6	-1.609212118	-3.539778254	0.262031019
11	7	-2.362082168	-2.423997176	-0.107995008
12	6	-0.200439015	-3.633814263	0.352998026
13	6	0.340476025	-4.989427360	0.639851046
14	6	0.133128010	-6.083101449	-0.214358016
15	9	-0.546080038	-5.924393413	-1.358541098
16	6	0.621833047	-7.355670549	0.074199005
17	9	0.403234029	-8.372046580	-0.767440057
18	6	1.354360095	-7.565762543	1.240079088
19	9	1.832503131	-8.779613606	1.522264110
20	6	1.586627113	-6.502125480	2.109935151
21	6	1.077369080	-5.243114377	1.807197128
22	9	1.324411097	-4.246182308	2.668161194
23	9	2.284557167	-6.700905463	3.233097230
24	6	0.670228048	-2.498468179	0.294088021
25	7	2.052465148	-2.582225185	-0.024983002
26	6	2.876429209	-3.631387260	-0.395828028
27	1	2.484377179	-4.623650335	-0.531576036
28	6	4.171069302	-3.183595228	-0.556012039
29	1	5.011527363	-3.800448273	-0.839158063
30	6	4.175988301	-1.788550129	-0.294951021
31	6	2.847893204	-1.441396105	0.014618001
32	6	2.363344171	-0.145399011	0.207295015
33	6	0.969122069	-0.013974001	0.418713030
34	6	0.228225017	-1.203207086	0.534271040
35	6	0.224595016	1.220163089	0.398766029
36	7	-1.090005076	1.177250085	0.285826020
37	6	-1.553065110	2.489355181	0.202941014
38	6	-2.914893208	2.749257200	-0.057051004
39	6	-3.868998280	1.723232124	-0.259878019
40	6	-5.238661377	1.809120132	-0.649752047
41	6	-5.739592388	0.528832038	-0.746518055
42	1	-6.740640483	0.249061018	-1.041584077
43	6	-4.700449337	-0.394782028	-0.411816030
44	7	-3.592446260	0.376513027	-0.137447010
45	1	-5.770603392	2.727677198	-0.852417059
46	6	-3.378020241	4.159180298	-0.166626012
47	6	-2.905275211	5.021078361	-1.164978083
48	9	-2.021763146	4.580727329	-2.072504148
49	6	-3.325323242	6.345197437	-1.264141089
50	9	-2.850621203	7.136394526	-2.233946162
51	6	-4.256696309	6.842409470	-0.356401026
52	6	-4.754525341	6.012596413	0.644895047
53	6	-4.311595310	4.695090338	0.730903051
54	9	-4.805369347	3.935940282	1.718386126
55	9	-5.644148392	6.488288447	1.523952111
56	9	-4.670511335	8.109181592	-0.445753032
57	6	-0.451440033	3.380291243	0.326386024
58	6	0.701733049	2.595968188	0.422778030
59	6	2.057764149	3.027933216	0.477973034

60	6	3.204390233	2.256360163	0.356391026
61	7	3.324858238	0.853015061	0.151334011
62	6	4.698200339	0.541231039	-0.058459004
63	6	5.143835370	-0.746475054	-0.314748023
64	6	6.570520475	-1.020176074	-0.602909044
65	6	7.259673510	-0.380497027	-1.643250116
66	9	6.635482486	0.526898038	-2.407355171
67	6	8.593304637	-0.658623048	-1.930462137
68	9	9.214484642	-0.027977002	-2.931803210
69	6	9.276416690	-1.611928115	-1.179279083
70	6	8.620739620	-2.274684164	-0.144179010
71	6	7.290044527	-1.974133140	0.131308009
72	9	6.699520500	-2.623797191	1.143855084
73	9	9.273775672	-3.184468228	0.585092043
74	9	10.552916783	-1.888077135	-1.448739106
75	6	5.426757404	1.763967125	0.068461005
76	6	4.548419327	2.768645201	0.325456024
77	6	2.261010160	4.505254323	0.619300045
78	6	2.657866193	5.303786401	-0.457922033
79	9	2.921224211	4.743047343	-1.645687120
80	6	2.801387202	6.684320466	-0.338789024
81	9	3.187397229	7.419224525	-1.386575099
82	6	2.535288184	7.299358523	0.882366063
83	9	2.670003191	8.620693634	1.008538075
84	6	2.133259152	6.531732471	1.973465144
85	6	1.998762145	5.152927371	1.831084131
86	9	1.614001114	4.442648321	2.898346206
87	9	1.884175135	7.120279491	3.147542229
88	6	-7.159006534	-2.166499156	0.450798033
89	6	-8.428213612	-2.724317198	0.316986023
90	6	-8.703507651	-3.557737254	-0.764378057
91	9	-9.915645714	-4.101015294	-0.899659067
92	9	-9.378021685	-2.476386179	1.226065088
93	9	-6.930807524	-1.385849100	1.514546107
94	1	-2.321847165	-5.538269391	0.937897066
95	1	-4.762989340	-4.583509330	0.506531037
96	1	6.500080474	1.843531132	-0.019198001
97	1	4.791715346	3.809458273	0.477216034
98	1	-0.493548035	4.459498319	0.298251021
99	1	-1.969580142	-1.662719119	-0.644291044
100	1	-0.787588057	-1.081526080	0.867857065
101	1	-2.665318189	0.103593007	0.181226013

Table S12. Atomic Cartesian coordinates for the porphyrinoid **4** optimized by the B3LYP/6-31G(d) method. First column contains atomic numbers.

1	9	-11.493084834	-0.192657110	-2.372378163
2	6	-10.212298776	-0.257939102	-2.006039136
3	6	-9.831721748	0.130283930	-0.723849044
4	9	-10.752037821	0.561245951	0.144561018
5	6	-8.491751660	0.058269937	-0.353171017
6	9	-8.168092619	0.430946967	0.893592071
7	6	-7.498985560	-0.392498085	-1.232357079
8	6	-7.915441599	-0.773715115	-2.514570175
9	6	-9.250377677	-0.711203126	-2.905588203
10	9	-9.610964716	-1.074302154	-4.140187290
11	9	-7.021170519	-1.200152140	-3.413992240
12	6	-6.075490452	-0.492291079	-0.819789054
13	6	-5.374987412	-1.703403160	-0.855296053
14	6	-5.712956410	-3.025909256	-1.221115079
15	1	-6.663041455	-3.384747291	-1.591468106
16	6	-4.559698322	-3.771124302	-0.997403063
17	1	-4.434556301	-4.835543378	-1.166161075
18	7	-3.512665254	-3.040551236	-0.513092029
19	6	-3.976071301	-1.780616153	-0.420903022
20	6	-3.291291260	-0.621457062	0.025390010
21	7	-4.056298329	0.533577014	0.025271010
22	6	-5.388339400	0.640803009	-0.369974019
23	6	-5.747002457	2.012886103	-0.213257007
24	1	-6.722575536	2.417897122	-0.441388024
25	6	-4.660085390	2.706458164	0.264053027
26	1	-4.602025396	3.761006243	0.491044043
27	6	-3.585712305	1.784107109	0.419904038
28	6	-2.267247213	1.907813128	0.845354067
29	6	-1.770432190	3.265604234	1.218202096
30	6	-1.281601161	4.147484301	0.250974026
31	9	-1.255767156	3.771318277	-1.038432065
32	6	-0.780934140	5.402592419	0.581837048
33	6	-0.779128143	5.807382428	1.914238145
34	6	-1.269520171	4.956186361	2.901820218
35	6	-1.757047191	3.701907267	2.545614189
36	9	-2.203956216	2.892871201	3.515512260
37	9	-1.269778171	5.346643408	4.179413311
38	9	-0.305727119	7.009440512	2.244924172
39	9	-0.294454111	6.213268469	-0.363770019
40	6	-1.438751140	0.766646058	0.867152069
41	6	-1.939222164	-0.495991039	0.468959041
42	6	-1.112370091	-1.683013119	0.492240043
43	1	-1.499517114	-2.542120180	-0.045608995
44	6	0.055707992	-1.815026115	1.176461092
45	16	0.696777024	-0.490979013	2.166999165
46	6	0.023611963	0.945032084	1.235768098
47	1	0.097967960	1.757156143	1.961236149
48	6	0.929661025	1.347583123	0.045748011
49	1	0.326308976	1.859109152	-0.718372043
50	1	1.394573068	0.492682064	-0.445139024
51	6	1.959336090	2.396475207	0.466417042
52	8	1.698634061	3.183187259	1.366977104
53	6	3.231869179	2.588988234	-0.303955014
54	6	3.567185190	4.012871340	-0.544664034
55	6	2.630362111	4.847027392	-1.172388078
56	9	1.466215032	4.323239342	-1.595809106
57	6	2.846010116	6.203964475	-1.373546089
58	9	1.928584044	6.957729522	-1.985820136
59	6	4.040451196	6.774860523	-0.936874060

60	9	4.270259201	8.075013622	-1.129044075
61	6	4.992128270	5.983306505	-0.299956014
62	6	4.746166267	4.626389393	-0.101265999
63	9	5.677197363	3.921452351	0.556603045
64	9	6.131121374	6.532647524	0.135643017
65	6	4.088287247	1.565195170	-0.623423040
66	7	3.883270249	0.235428070	-0.270808012
67	6	4.986620334	-0.428699967	-0.632617039
68	6	5.188796360	-1.825931067	-0.401765021
69	6	4.192078300	-2.624021133	0.162678019
70	7	2.962888204	-2.162754111	0.534751047
71	6	2.128175156	-3.202276196	0.921008072
72	6	0.779792054	-3.097135201	1.171335090
73	6	-0.044612991	-4.318791295	1.344092104
74	6	-0.860582047	-4.467027316	2.476361186
75	6	-1.698774097	-5.561984417	2.649213198
76	9	-2.447781148	-5.678268418	3.750035276
77	6	-1.745889092	-6.551615459	1.668953128
78	9	-2.542700137	-7.610158556	1.825549138
79	6	-0.954999037	-6.436031453	0.529271046
80	9	-1.007861029	-7.378734528	-0.418210022
81	6	-0.124037987	-5.329484360	0.375834035
82	9	0.593175062	-5.243786358	-0.754197047
83	9	-0.828834053	-3.539041247	3.440829257
84	6	2.949688227	-4.401239275	0.857642071
85	1	2.606664209	-5.389463373	1.127537089
86	6	4.181074308	-4.058327237	0.401142037
87	1	5.017355377	-4.718103277	0.221333024
88	1	2.753963178	-1.165443040	0.468836041
89	6	6.477477462	-2.462723097	-0.785764047
90	6	7.329339536	-3.033918131	0.168937020
91	9	6.989602503	-3.013742132	1.466094115
92	6	8.534743607	-3.640026163	-0.176521005
93	9	9.319598665	-4.174365192	0.765342065
94	6	8.927694651	-3.678134164	-1.512022101
95	6	8.108580605	-3.116937130	-2.489029171
96	6	6.901266469	-2.530398099	-2.119477143
97	9	6.134175415	-2.012138068	-3.090383217
98	9	8.477579605	-3.159081129	-3.773876262
99	9	10.083474755	-4.250999192	-1.854700126
100	6	5.956983376	0.475788108	-1.283090085
101	6	5.394427320	1.699234190	-1.291767084
102	1	5.804792370	2.611476262	-1.700137115
103	1	6.922338466	0.193329096	-1.679034114

Table S13. Atomic Cartesian coordinates for the porphyrinoid **5** optimized by the B3LYP/6-31G(d) method. First column contains atomic numbers.

1	9	-9.899496706	-1.337384094	1.545929112
2	6	-9.057448648	-1.807796131	0.618730047
3	9	-10.813743804	-3.018989216	-0.400013029
4	6	-9.525184661	-2.670669193	-0.369141026
5	6	-8.643158637	-3.168015229	-1.325299094
6	9	-9.090720667	-3.989098285	-2.282198163
7	6	-7.302718533	-2.794201203	-1.286154090
8	6	-7.710632540	-1.454897105	0.645123048
9	9	-7.301854546	-0.642317049	1.628634119
10	6	-6.794689483	-1.929086138	-0.305517022
11	9	-6.494457490	-3.279621235	-2.238064161
12	6	-5.355884378	-1.561975111	-0.269726020
13	6	-4.416192316	-2.609366188	-0.123945009
14	6	-4.563748328	-3.945097281	0.324125023
15	6	-3.299596237	-4.519199324	0.417468030
16	6	-2.340881168	-3.554504256	0.030402002
17	7	-3.056295222	-2.419317175	-0.307466022
18	6	-0.917615067	-3.528106255	0.095427007
19	9	0.681034048	-4.000841289	2.404379173
20	6	0.551550038	-4.995260359	1.517404109
21	6	1.195189088	-6.198784464	1.794229127
22	9	1.910839138	-6.344266456	2.914330212
23	6	1.082227075	-7.261706503	0.900501062
24	6	-0.304951022	-5.897115438	-0.519161038
25	6	-0.208664015	-4.804580344	0.354307025
26	9	-1.015163072	-5.791247390	-1.649989120
27	6	0.328929023	-7.110906492	-0.262035019
28	9	0.220995016	-8.128984569	-1.122633082
29	9	1.693366123	-8.420564620	1.156730083
30	6	-0.308856022	-2.276813166	0.034353002
31	6	0.990436069	-1.778737129	0.014563001
32	7	2.243293163	-2.475404179	-0.048038003
33	6	2.914719210	-3.663593263	-0.362351026
34	1	2.384624172	-4.587597330	-0.526068038
35	6	4.280773307	-3.425482244	-0.413998030
36	1	5.024505361	-4.184777300	-0.611029042
37	6	4.501117321	-2.019167145	-0.158976011
38	6	3.216870232	-1.545800109	0.057071004
39	6	2.720107196	-0.272749020	0.136179010
40	6	1.302124094	-0.362804026	0.115761008
41	6	0.459835033	0.800200055	0.141042010
42	7	-0.864867060	0.793339055	0.047623003
43	6	-1.286045090	2.132731155	0.040657003
44	6	-2.630870190	2.547141183	-0.138847010
45	6	-3.745252271	1.707340122	-0.282080020
46	7	-3.732863268	0.331466024	-0.155368011
47	6	-5.002755361	-0.203090015	-0.345417025
48	6	-5.847180420	0.913245063	-0.644034044
49	1	-6.896203512	0.836367060	-0.891907065
50	6	-5.095181369	2.060673147	-0.603229043
51	1	-5.437338409	3.064981222	-0.807181057
52	6	-2.898045210	4.014638289	-0.207692015
53	9	-4.054802292	3.996309288	1.864867135
54	6	-3.606409258	4.677624335	0.802176056
55	6	-2.460364179	4.796332344	-1.284144090
56	9	-1.784616130	4.230828304	-2.293761168
57	6	-3.869544280	6.044671433	0.750446053
58	9	-4.548024328	6.643973452	1.735822124
59	6	-3.413529247	6.791923473	-0.332404024

60	6	-2.703156193	6.166028446	-1.353899097
61	9	-3.656294263	8.103972583	-0.391654028
62	9	-2.269655165	6.880593472	-2.399524173
63	6	-0.175495013	2.986995217	0.180666013
64	6	0.979102072	2.197012157	0.234685017
65	6	2.299582165	2.727471195	0.324929023
66	6	3.527352251	2.069938146	0.271779019
67	7	3.680993267	0.686358048	0.137932010
68	6	5.053317363	0.334345024	0.037348003
69	6	5.493062414	-0.998747073	-0.152231011
70	6	6.928031513	-1.303686093	-0.348523025
71	6	7.557084565	-2.311570168	0.398526029
72	9	6.868205485	-2.980634216	1.333928096
73	6	8.894346642	-2.649520190	0.215498015
74	9	9.456891691	-3.608985261	0.956390070
75	6	9.650840709	-1.975210143	-0.740252052
76	6	9.059384643	-0.973165068	-1.505276107
77	6	7.717407544	-0.657470050	-1.311397094
78	9	7.185665531	0.291163021	-2.095922152
79	9	9.775346697	-0.333382024	-2.435082175
80	9	10.934216773	-2.288392167	-0.922341065
81	6	5.761050420	1.572905113	0.155036011
82	6	4.860737348	2.596617187	0.296456021
83	6	2.403621174	4.218081303	0.461259033
84	9	1.800459130	4.128332296	2.750871196
85	6	2.139191155	4.853651347	1.678095120
86	6	2.754988200	5.028502364	-0.621827046
87	9	3.022839218	4.475770324	-1.812042132
88	6	2.219346162	6.237055463	1.817349129
89	9	1.965590140	6.816503492	2.994866216
90	6	2.572793188	7.018924479	0.719375051
91	6	2.843301205	6.414161457	-0.505939037
92	9	3.184212228	7.162765492	-1.559417110
93	9	2.655449192	8.344768604	0.842813058
94	1	-5.500361408	-4.400370318	0.614387042
95	1	-3.069070222	-5.505219414	0.796516055
96	1	5.097339365	3.644937262	0.404791029
97	1	6.836610481	1.665611120	0.132174010
98	1	-0.209403015	4.065003295	0.214873016
99	1	-2.688957193	-1.710295122	-0.925641067
100	1	-2.925447209	-0.135186010	0.237232017
101	1	-0.990880070	-1.437011104	0.051988004

Table S14. Atomic Cartesian coordinates for the porphyrinoid **1** taken from the single crystal X-ray data. First column contains atomic numbers.

1	9	-9.042272373	-4.659915079	0.013456119
2	6	-7.902496494	-3.895707581	-0.156576556
3	6	-7.607094302	-2.973858360	0.833481933
4	9	-8.417010083	-2.777894870	1.898867763
5	6	-6.426700418	-2.238010281	0.688567437
6	9	-6.123553346	-1.366430157	1.662813407
7	6	-5.530987012	-2.374892697	-0.413780495
8	6	-5.940914539	-3.305744133	-1.370855370
9	6	-7.104351573	-4.075964387	-1.225802621
10	9	-7.393480211	-4.965075713	-2.194935702
11	9	-5.216252139	-3.453722566	-2.494260940
12	6	-4.309036796	-1.581739632	-0.493355791
13	6	-3.086076201	-2.179800857	-0.776889623
14	6	-2.754427553	-3.575809800	-0.961891000
15	1	-3.371976630	-4.305008413	-0.864035733
16	6	-1.470125085	-3.692473201	-1.256071338
17	1	-0.992603542	-4.493458513	-1.464821994
18	6	-0.881206820	-2.379171931	-1.257234220
19	7	-1.906079036	-1.510372645	-0.952678780
20	1	-1.807698693	-0.633510455	-0.891595898
21	6	0.316733792	-2.077563289	-1.440427393
22	6	1.331124695	-3.157623659	-1.707181988
23	6	1.742754241	-4.032726420	-0.709894894
24	9	1.269265790	-3.897172757	0.499005079
25	6	2.643558204	-5.036124596	-0.903444859
26	9	3.099198855	-5.796387554	0.043247309
27	6	3.210529377	-5.181579334	-2.173769184
28	9	4.167268799	-6.107191079	-2.423732789
29	6	2.805416405	-4.348059443	-3.184033181
30	6	1.928004908	-3.341813622	-2.967209116
31	9	1.557782291	-2.537232191	-3.957999300
32	9	3.356441483	-4.478108912	-4.462256862
33	6	0.847832315	-0.714389699	-1.617643208
34	6	0.220395955	0.454708110	-1.959263159
35	1	-0.720782155	0.526801073	-2.086650363
36	6	1.101820588	1.540427225	-2.079587318
37	6	2.422508918	1.225933852	-1.851805575
38	16	2.576782099	-0.445071113	-1.461689402
39	6	3.624939167	2.072148377	-1.925343273
40	6	4.761775138	2.127374161	-1.121774132
41	6	5.052322118	1.404976296	0.121261301
42	6	4.129720402	1.085868334	1.133615722
43	6	4.321298119	0.211291701	2.213830040
44	6	3.143324898	0.077371673	2.782103533
45	1	2.969121515	-0.477343574	3.521065848
46	6	2.105314593	0.870490796	2.171600489
47	6	0.865149328	1.078068689	2.259655943
48	6	0.153625005	0.168399121	3.199014623
49	6	0.149306201	-1.231881608	3.130549268
50	6	-0.525657667	-2.057878615	3.998003587
51	9	-0.502039471	-3.391169031	3.841875105
52	6	-1.240394784	-1.519631988	5.020630931
53	9	-1.926434336	-2.332024461	5.883932415
54	6	-1.303773730	-0.155602367	5.153539073
55	9	-2.044364100	0.384254768	6.152628884
56	6	-0.628012361	0.654061360	4.279332866
57	9	-0.740839973	1.970408828	4.488570841
58	9	0.851351233	-1.788428714	2.087599427
59	6	0.099258274	2.067540624	1.560870945

60	7	-1.186062611	1.854450746	1.124017203
61	1	-1.632995682	1.115786798	1.233079158
62	6	-1.658150398	2.976370624	0.472626241
63	6	-2.937333303	3.031751447	-0.124495472
64	6	-3.782254852	1.936726098	-0.263489512
65	7	-3.321760212	0.638026247	-0.138151289
66	6	-4.407881799	-0.149243278	-0.362309407
67	6	-5.612741087	0.635018303	-0.554912959
68	1	-6.505904652	0.305038410	-0.677196534
69	6	-5.189248579	1.952033714	-0.565049815
70	1	-5.793517825	2.688146419	-0.649772479
71	6	-3.403160172	4.309753604	-0.698329180
72	6	-4.213344426	5.227091599	-0.025222388
73	9	-4.579661158	4.988518625	1.257165713
74	6	-4.674987677	6.369136464	-0.657563508
75	9	-5.485777601	7.235602560	-0.008387484
76	6	-4.401206932	6.567016263	-1.900872778
77	6	-3.601556713	5.682527343	-2.568786051
78	6	-3.155326463	4.549303641	-1.946867314
79	9	-2.399991828	3.680489897	-2.649195968
80	9	-3.258095072	5.924582912	-3.871036597
81	9	-4.851889674	7.670944776	-2.540425844
82	6	-0.726730234	3.904294620	0.616107238
83	6	0.376849911	3.348764571	1.252630220
84	1	1.171255258	3.760285117	1.464283487
85	1	-0.767036501	4.789501914	0.261468568
86	7	2.843306026	1.531075758	1.142707664
87	1	2.474404013	2.123540812	0.634391249
88	1	5.128088738	-0.202179301	2.492233990
89	6	6.436359807	1.008300479	0.370789516
90	6	7.143973667	0.135948620	-0.522636538
91	9	6.420401727	-0.471256930	-1.480945082
92	6	8.436015272	-0.207268585	-0.334946023
93	9	9.041953756	-1.078754561	-1.178790223
94	6	9.196034295	0.384190446	0.650356273
95	6	8.592347620	1.266766216	1.501407811
96	6	7.220240332	1.564395700	1.362258457
97	9	6.700099473	2.494962750	2.169140555
98	9	9.276314135	1.808457004	2.537099955
99	9	10.464960645	0.067119336	0.828347898
100	6	5.640076585	3.074342246	-1.742733322
101	6	5.002112712	3.567229964	-2.838759816
102	7	3.783549617	2.979269076	-2.951095208
103	1	3.188300445	3.150776147	-3.575955081
104	1	5.325737943	4.202103325	-3.400598446
105	1	6.488083656	3.306545932	-1.418433136
106	1	0.844673889	2.425399083	-2.348632885

Table S15. Atomic Cartesian coordinates for the porphyrinoid **2** taken from the single crystal X-ray data. First column contains atomic numbers.

1	9	2.625509360	-6.314951782	3.932338691
2	6	1.869843412	-5.598519819	3.000522993
3	6	1.082518081	-6.312835338	2.153090747
4	9	1.060070620	-7.662183029	2.173269746
5	6	0.318398487	-5.593385689	1.222470662
6	9	-0.427145153	-6.314280574	0.375090296
7	6	0.282396732	-4.227293326	1.207611926
8	6	1.078377920	-3.587246845	2.126382695
9	6	1.867649237	-4.227729173	2.992873567
10	9	2.586103355	-3.571888317	3.914112789
11	9	1.071781228	-2.248794458	2.218572425
12	6	-0.615991296	-3.516824402	0.255281528
13	6	-2.015280402	-3.710963596	0.204054088
14	6	-2.997153817	-4.498408066	0.887250326
15	1	-2.849667297	-5.245129685	1.481222287
16	6	-4.224799134	-3.969288947	0.508541717
17	1	-5.062508013	-4.321431641	0.778659265
18	6	-4.070046169	-2.865620504	-0.289612254
19	7	-2.679041576	-2.742404847	-0.536985270
20	16	-1.640490732	-1.859091737	-1.515569197
21	6	-0.277207081	-2.438801180	-0.540259454
22	6	0.940293001	-1.722693464	-0.630307144
23	7	2.202489660	-2.374919611	-0.706109149
24	6	2.892671352	-3.574558439	-0.991595052
25	1	2.490171659	-4.415379664	-1.144878439
26	6	4.236702283	-3.321802091	-1.028205894
27	1	4.925389674	-3.917621917	-1.252434652
28	6	4.446438458	-1.868094587	-0.828958410
29	6	5.399583147	-0.939578643	-0.673730767
30	6	6.845659783	-1.172487812	-0.922586095
31	6	7.482949214	-2.197998485	-0.348758369
32	9	6.809392355	-2.971806968	0.502761931
33	6	8.815007785	-2.520499865	-0.551201236
34	9	9.395279637	-3.487717071	0.057823977
35	6	9.530841354	-1.781902482	-1.423089716
36	9	10.810979170	-2.106947692	-1.633263462
37	6	8.941620903	-0.783035868	-2.010499259
38	6	7.618013187	-0.456844582	-1.804455302
39	9	7.068947604	0.548376318	-2.506216102
40	9	9.626791879	-0.062522882	-2.898812253
41	6	4.948262603	0.375314996	-0.402089875
42	7	3.577624608	0.719437896	-0.312044249
43	6	2.629023234	-0.266358121	-0.384251695
44	6	3.161680474	-1.467244551	-0.565097764
45	6	1.219611591	-0.343932305	-0.476736079
46	6	0.369103664	0.789728267	-0.256690022
47	7	-0.940597299	0.777829992	-0.290852389
48	6	-1.394562305	2.064062877	-0.040009760
49	6	-0.306162058	2.951003634	0.100884789
50	6	0.867160149	2.142341649	0.026553855
51	6	2.157280307	2.696491338	0.075883104
52	6	3.412039597	2.092231056	-0.089929805
53	6	4.727273919	2.649966699	-0.035176543
54	6	5.637634591	1.608186038	-0.182698580
55	1	6.588243838	1.751998369	-0.218549207
56	1	4.938723120	3.554292025	0.141769993
57	6	2.239482626	4.206550536	0.300910509
58	6	2.621572741	4.681074771	1.548050907
59	9	2.976326612	3.865174980	2.486551023

60	6	2.653049283	6.053367721	1.792244754
61	9	3.011005360	6.490519035	3.009909497
62	6	2.273164414	6.905926986	0.877100855
63	6	1.885751681	6.454572183	-0.354075607
64	6	1.863976418	5.148462507	-0.673300557
65	9	1.439594209	4.746041063	-1.873690901
66	9	1.514604809	7.366856192	-1.348979199
67	9	2.307306475	8.256573860	1.106117677
68	1	-0.360178707	3.835798562	0.357105896
69	6	-2.778636099	2.362963666	-0.107302763
70	6	-3.778079109	1.434585150	-0.391171179
71	7	-3.604612272	0.105930818	-0.457354085
72	1	-2.882335869	-0.127933227	-0.295432832
73	6	-4.781062320	-0.516209167	-0.789300459
74	6	-5.023820341	-1.874092456	-0.676842483
75	6	-6.434651729	-2.351913106	-0.808795497
76	6	-6.771044891	-3.369369612	-1.698213376
77	9	-5.837679572	-3.981562790	-2.400163446
78	6	-8.085042801	-3.831074036	-1.807615305
79	9	-8.354268394	-4.758597460	-2.748536201
80	6	-9.087717110	-3.220295507	-1.114568362
81	6	-8.780822352	-2.282362462	-0.161913921
82	6	-7.470928582	-1.823791794	-0.055220431
83	9	-7.248075373	-0.884313763	0.888970084
84	9	-9.750893575	-1.674120380	0.533031189
85	9	-10.347818953	-3.617988011	-1.295522285
86	6	-5.733959879	0.523778696	-1.018306533
87	6	-5.145082080	1.666924554	-0.751058068
88	1	-5.555104848	2.565345907	-0.896028959
89	1	-6.640953914	0.361893511	-1.237350195
90	6	-3.216163850	3.777358407	0.113600641
91	6	-3.942066329	4.099957299	1.249402482
92	9	-4.262258173	3.193973273	2.046629143
93	6	-4.364158746	5.398094148	1.512387361
94	9	-5.057188872	5.651856970	2.602702873
95	6	-4.031143015	6.410535905	0.669288033
96	6	-3.326989515	6.122047942	-0.444595177
97	6	-2.916729956	4.822769775	-0.709743565
98	9	-2.212311751	4.643977255	-1.868613916
99	9	-3.021496860	7.116434330	-1.303740815
100	9	-4.418928676	7.674677857	0.911867112

Table S16. Atomic Cartesian coordinates for the porphyrinoid **3** taken from the single crystal X-ray data. First column contains atomic numbers.

1	9	-8.506558410	-3.985335036	-2.584706582
2	6	-8.036823482	-3.332296681	-1.491994711
3	6	-6.730043020	-2.795183149	-1.450919893
4	9	-5.976128110	-2.944439693	-2.556206751
5	6	-6.230837577	-2.156424923	-0.375429238
6	6	-4.806843000	-1.590762840	-0.306500650
7	6	-3.813319203	-2.552814281	-0.228874856
8	6	-3.959278268	-3.951767566	0.036423010
9	1	-4.771125642	-4.410445546	0.103112427
10	6	-2.747373445	-4.529711578	0.158278186
11	6	-1.712964705	-3.493357259	0.035361140
12	7	-2.444318011	-2.322448655	-0.224668981
13	1	-2.034175210	-1.660365502	-0.617471590
14	6	-0.360224390	-3.661033818	0.113364227
15	6	0.154967727	-5.031409409	0.373919669
16	6	-0.092203020	-6.075086584	-0.568022415
17	9	-0.721335431	-5.830068627	-1.700677648
18	6	0.371674801	-7.360375094	-0.307659148
19	9	0.120002621	-8.339770578	-1.278089911
20	6	1.027093003	-7.670327596	0.835792517
21	9	1.487997592	-8.905173132	1.073337713
22	6	1.289431560	-6.666635785	1.785225245
23	6	0.833736547	-5.388653890	1.521754824
24	9	0.988158300	-4.513825153	2.346795920
25	9	1.887531918	-6.988255377	2.842819214
26	6	0.575128170	-2.547874781	0.173012007
27	7	1.928160136	-2.706350990	-0.171184260
28	6	2.787015092	-3.748593766	-0.498443240
29	1	2.496236390	-4.617205877	-0.657345307
30	6	3.987915383	-3.397015778	-0.694161507
31	1	4.742770547	-3.934672537	-0.910015664
32	6	4.065049979	-2.002251122	-0.343967128
33	6	2.719266587	-1.631423507	-0.112177915
34	6	2.295448042	-0.320787500	0.138084704
35	6	0.913035694	-0.132513184	0.352535572
36	6	0.161572031	-1.280310846	0.436369663
37	1	-0.740635388	-1.164935241	0.707486566
38	6	0.239235888	1.132854860	0.414912067
39	7	-1.125860661	1.107021506	0.304983388
40	6	-1.529138313	2.447291331	0.245173561
41	6	-2.781805072	2.834952550	0.113272048
42	6	-3.786948289	1.882812107	-0.108450678
43	6	-5.174906203	2.029063855	-0.424818415
44	6	-5.752161671	0.762216448	-0.564543419
45	1	-6.635855609	0.593242167	-0.722713636
46	6	-4.737544868	-0.207738502	-0.361288714
47	7	-3.536496476	0.532615568	-0.056369195
48	1	-2.752198801	0.312122670	0.100952555
49	1	-5.602506429	2.872949101	-0.493998237
50	6	-3.100212494	4.295812837	0.061946903
51	6	-2.565916778	5.120649406	-0.932456436
52	9	-1.771805267	4.608801674	-1.889295020
53	6	-2.818940112	6.458384006	-0.976166053
54	9	-2.198761569	7.248825376	-1.885257546
55	6	-3.622817314	7.019624422	-0.036000682
56	6	-4.189727838	6.255886394	0.954763654
57	6	-3.974550440	4.877853348	0.910856362
58	9	-4.552887912	4.140921630	1.897639865
59	9	-4.982161460	6.794873636	1.896614484

60	9	-3.807785109	8.369628346	-0.003036247
61	6	-0.371235920	3.295531727	0.392603495
62	6	0.753193759	2.479814845	0.427733973
63	6	2.105384772	2.862405885	0.369563203
64	6	3.221721719	2.069513646	0.260834214
65	7	3.331261642	0.677103902	0.172395628
66	6	4.662980026	0.302408162	-0.045821061
67	6	5.066471090	-0.997719443	-0.284535219
68	6	6.492670934	-1.300288838	-0.477931536
69	6	7.241428537	-0.759452989	-1.507416312
70	9	6.689228638	0.010508461	-2.410298296
71	6	8.618139507	-0.943476716	-1.580165272
72	9	9.324167317	-0.387765372	-2.581759435
73	6	9.266028253	-1.699753239	-0.624176107
74	6	8.545885487	-2.272992093	0.397876697
75	6	7.180613317	-2.069314818	0.451315243
76	9	6.529376891	-2.570254799	1.519256970
77	9	9.171333889	-2.992101063	1.353802882
78	9	10.604898235	-1.870367879	-0.672343476
79	6	5.458198153	1.518032973	0.078395397
80	6	4.613724102	2.555039100	0.257267144
81	1	4.855208493	3.447512671	0.305870964
82	1	6.379706620	1.561629997	-0.010117616
83	6	2.362034420	4.380755935	0.370222142
84	6	1.985340336	5.084358440	-0.783696123
85	9	1.555521196	4.424052313	-1.905783284
86	6	2.048635053	6.466242817	-0.832947083
87	9	1.668585197	7.115566321	-1.956889847
88	6	2.481881293	7.157133723	0.270978960
89	9	2.529449750	8.512563619	0.247992900
90	6	2.864402878	6.492953356	1.400322092
91	6	2.803458672	5.106246910	1.450045158
92	9	3.184706336	4.482295418	2.560282972
93	9	3.312657649	7.186694199	2.490405381
94	1	-0.361403732	4.251715184	0.461781937
95	1	-2.523100190	-5.412445488	0.415111752
96	6	-7.021165121	-2.034916741	0.773882060
97	6	-8.336575194	-2.557384822	0.732606451
98	6	-8.806552590	-3.190353552	-0.369961962
99	9	-10.038815476	-3.674936775	-0.359883139
100	9	-9.093850698	-2.420500542	1.846872933
101	9	-6.616645522	-1.481015696	1.831100938

Table S17. Atomic Cartesian coordinates for the porphyrinoid **4** taken from the single crystal X-ray data. First column contains atomic numbers.

1	9	11.482414398	0.212197842	2.078417460
2	6	10.238761078	0.000841868	1.646370807
3	6	9.912494358	0.307740841	0.315895578
4	9	10.857588150	0.670961577	-0.455770574
5	6	8.620534140	0.099042599	-0.109489112
6	9	8.334294017	0.250640923	-1.314279861
7	6	7.616970496	-0.339190162	0.733307013
8	6	7.985372055	-0.638397883	2.073082867
9	6	9.270662364	-0.432109263	2.495195535
10	9	9.589596116	-0.647384228	3.783229380
11	9	7.062842751	-1.044376376	2.960129344
12	6	6.203393387	-0.449222625	0.282380294
13	6	5.533790964	-1.732270768	0.374935091
14	6	5.938529907	-2.999772117	0.613205902
15	1	6.805604875	-3.293925573	0.846239931
16	6	4.797509552	-3.748295590	0.451578570
17	1	4.792699489	-4.729989292	0.600291332
18	7	3.674998895	-3.055873150	0.109148634
19	6	4.117476760	-1.768316105	0.035858343
20	6	3.368681729	-0.660379980	-0.243270328
21	7	4.127388853	0.430148596	-0.269022630
22	6	5.492791740	0.537522962	-0.000636821
23	6	5.803224630	1.901524111	-0.132445690
24	1	6.660805893	2.346359640	-0.051415713
25	6	4.677876784	2.594411153	-0.474018589
26	1	4.621711980	3.554573139	-0.651893861
27	6	3.592064284	1.669424466	-0.542743660
28	6	2.239695879	1.804379021	-0.808335906
29	6	1.675701435	3.138230625	-0.937701572
30	6	1.516559225	3.973761294	0.151274341
31	9	1.873154384	3.481591791	1.381549656
32	6	0.953377210	5.224060361	0.076893363
33	6	0.534538074	5.716500734	-1.149559054
34	6	0.677089101	4.965939166	-2.290515591
35	6	1.263839802	3.728706221	-2.197701119
36	9	1.392702739	2.993226285	-3.315137860
37	9	0.235518767	5.385686106	-3.444297803
38	9	-0.036343238	6.862462695	-1.199867369
39	9	0.796963628	5.955297206	1.189435359
40	6	1.425663369	0.689642672	-0.816096079
41	6	1.979006746	-0.526903619	-0.509048045
42	6	1.164268711	-1.698680036	-0.421713869
43	1	1.518315172	-2.443231859	0.065334187
44	6	-0.061008879	-1.854722246	-0.952430289
45	16	-0.774579272	-0.683849885	-1.863155601
46	6	-0.047634173	0.808797857	-1.098908240
47	1	-0.091074771	1.538630795	-1.806383995
48	6	-0.938425486	1.300268491	0.054273357
49	1	-0.381660843	1.766473510	0.727575034
50	1	-1.382143690	0.591179910	0.457446600
51	6	-1.997611481	2.320084651	-0.522037663
52	8	-1.763746247	2.982287545	-1.527995713
53	6	-3.286233728	2.522431468	0.216468122
54	6	-3.597451980	3.959090538	0.409618889
55	6	-2.687106237	4.780489396	1.056260073
56	9	-1.553486086	4.276473721	1.501351967
57	6	-2.872866232	6.173841959	1.177149006
58	9	-1.948642307	6.875113841	1.822841026
59	6	-4.026247094	6.688097257	0.748599918

60	9	-4.222260861	8.071456122	0.854963508
61	6	-4.954278989	5.963519668	0.067931592
62	6	-4.738122365	4.648608985	-0.117369427
63	9	-5.620585135	3.906647273	-0.826782263
64	9	-6.044585865	6.543278430	-0.446355301
65	6	-4.183763031	1.579535175	0.472717978
66	7	-3.947447770	0.215799323	0.212598956
67	6	-5.083796359	-0.367693492	0.481035673
68	6	-5.257837036	-1.776249319	0.356928420
69	6	-4.212852296	-2.586836287	-0.018295428
70	7	-2.955633649	-2.132236342	-0.306783596
71	6	-2.122137270	-3.164327191	-0.642476225
72	6	-0.781805150	-3.138141750	-0.857628265
73	6	0.075283469	-4.355484673	-0.930783103
74	6	0.997610310	-4.429686510	-1.999245818
75	6	1.941466753	-5.471012127	-1.992593018
76	9	2.832286047	-5.516708752	-3.016292714
77	6	1.964249527	-6.364843513	-0.988065461
78	9	2.887499136	-7.388787255	-0.954040629
79	6	1.064470787	-6.304839629	0.057725635
80	9	1.122867883	-7.182908306	1.084097114
81	6	0.136691737	-5.266146775	0.046216292
82	9	-0.691858522	-5.196795800	1.102212110
83	9	1.009819509	-3.541585219	-3.014343494
84	6	-2.952181276	-4.345853653	-0.569022396
85	1	-2.665739293	-5.273770362	-0.717436389
86	6	-4.183411821	-4.018207690	-0.188008340
87	1	-4.921674209	-4.575298764	-0.082716808
88	1	-2.756717726	-1.314148980	-0.350802086
89	6	-6.584377087	-2.379957770	0.605276806
90	6	-7.281833019	-3.051327909	-0.370050140
91	9	-6.820731565	-3.036660497	-1.641388254
92	6	-8.439046717	-3.776105866	-0.132599850
93	9	-9.055783168	-4.363267341	-1.166392775
94	6	-8.950122559	-3.794262540	1.136211442
95	6	-8.316926419	-3.108867669	2.136236335
96	6	-7.141544955	-2.417414164	1.847478979
97	9	-6.533867595	-1.822932796	2.892819760
98	9	-8.827902776	-3.142215319	3.382108040
99	9	-10.094485187	-4.407959689	1.359487622
100	6	-6.094236397	0.538790320	0.999142204
101	6	-5.537840599	1.667701238	1.042432872
102	1	-5.944473626	2.535382240	1.287670231
103	1	-6.984385027	0.410327792	1.216362988

Table S18. Atomic Cartesian coordinates for the porphyrinoid **5** taken from the single crystal X-ray data. First column contains atomic numbers.

1	6	3.228484519	-1.268944246	-0.410583736
2	6	2.703548473	-0.052735342	-0.196237218
3	6	1.298238546	-0.212366447	-0.036954470
4	6	1.063224352	-1.641002912	-0.124640235
5	6	3.052672930	-3.418484928	-0.583108359
6	1	2.687766259	-4.295392400	-0.628611279
7	6	4.385204913	-3.108975320	-0.672702877
8	1	5.091474398	-3.731694284	-0.811105255
9	6	4.541640408	-1.693957870	-0.522607173
10	6	5.492753321	-0.660919158	-0.359372399
11	6	5.005959757	0.651812246	-0.192004529
12	6	5.631706324	1.916313313	0.006276477
13	1	6.569774070	2.056950300	0.021535407
14	6	4.704080927	2.892671971	0.169161577
15	1	4.892641719	3.811523852	0.322571827
16	6	3.397386938	2.313945565	0.073264057
17	6	2.155093598	2.896849222	0.172628760
18	6	0.402751624	0.894767072	0.015792695
19	6	0.838545852	2.312686869	0.070226474
20	6	-0.356708267	3.032966750	0.022768663
21	1	-0.437875579	3.978139347	0.046001667
22	6	-1.411878709	2.114284708	-0.065250030
23	6	-0.178341982	-2.213374069	0.060346747
24	1	-0.846824629	-1.563771186	0.241792865
25	6	-0.697899853	-3.499921116	0.047647480
26	6	-2.101636731	-3.624001766	0.053715388
27	6	-3.002489903	-4.671108342	0.337510238
28	1	-2.761960428	-5.573424170	0.505839965
29	6	-4.270216734	-4.178829824	0.329749665
30	1	-5.057973467	-4.685607762	0.492785000
31	6	-4.231895861	-2.810387369	0.046494415
32	6	-5.208623430	-1.828626976	-0.035259703
33	6	-4.976777986	-0.432279654	-0.108605510
34	6	-5.886443679	0.590245108	-0.414211305
35	1	-6.818015986	0.474718852	-0.553291629
36	6	-5.214902240	1.776986119	-0.480164039
37	1	-5.601271964	2.623070419	-0.673988154
38	6	-3.848322817	1.533939961	-0.209263647
39	6	-2.775003022	2.430971346	-0.195110123
40	6	6.920399560	-1.034281680	-0.190436887
41	6	7.979973282	-0.381775307	-0.835587307
42	6	9.292257770	-0.781216340	-0.674855570
43	6	9.601378459	-1.845146620	0.117508331
44	6	8.575367327	-2.508333345	0.775511566
45	6	7.290837128	-2.083117195	0.642118898
46	9	6.366417868	-2.734676097	1.353611601
47	9	8.865814304	-3.558584462	1.557039030
48	9	10.858091080	-2.248517058	0.235158865
49	9	10.253633287	-0.117211322	-1.319312205
50	9	7.736010135	0.642161751	-1.639650785
51	7	2.324565872	-2.255468616	-0.414851903
52	7	3.617070640	0.952411403	-0.135402670
53	7	-0.925656651	0.807525482	-0.030670916
54	7	-2.887586715	-2.503673156	-0.118195303
55	1	-2.638166793	-1.939455255	-0.601168395
56	7	-3.743133964	0.180178913	-0.000216907
57	1	-3.160136711	-0.206343045	0.339360857
58	6	-3.132681021	3.882989478	-0.312303442
59	6	-2.915345613	4.607480488	-1.467126772

60	6	-3.216204649	5.946055072	-1.592425531
61	6	-3.745907821	6.607039949	-0.522695891
62	6	-4.006172020	5.939537673	0.648800528
63	6	-3.712964823	4.596905050	0.739166233
64	9	-2.370390267	3.987488877	-2.532312530
65	9	-2.971556889	6.591707197	-2.736191327
66	9	-4.019254731	7.919403813	-0.603400089
67	9	-4.522322136	6.597289065	1.689395065
68	9	-3.990724044	3.973570261	1.878847506
69	6	2.149756655	4.401967428	0.352689351
70	6	2.380094287	5.298086739	-0.666092607
71	6	2.297782830	6.666721830	-0.505334042
72	6	1.997882123	7.184080169	0.736159919
73	6	1.798405346	6.316015111	1.775808170
74	6	1.875254413	4.949571984	1.598621450
75	9	2.631810554	4.858215813	-1.902801100
76	9	2.475566250	7.489513975	-1.531457490
77	9	1.904237779	8.495391553	0.918550039
78	9	1.526014400	6.810664974	3.003805083
79	9	1.663793830	4.140255215	2.643031794
80	6	0.102458713	-4.741933595	0.042910773
81	6	0.252602565	-5.527959589	-1.091708143
82	6	1.012681210	-6.664808166	-1.108395039
83	6	1.651742072	-7.037738371	0.032240369
84	6	1.512488735	-6.324537934	1.182292054
85	6	0.761699457	-5.165560017	1.174510370
86	9	-0.364733653	-5.164179113	-2.228242997
87	9	1.185695701	-7.360361070	-2.244852119
88	9	2.430448148	-8.144460833	0.021969204
89	9	2.149270203	-6.678482318	2.306282729
90	9	0.630494409	-4.476529693	2.312450983
91	6	-6.608165668	-2.326317872	0.019101280
92	6	-7.295295447	-2.386187467	1.214267986
93	6	-8.561921674	-2.867749654	1.316464411
94	6	-9.217628379	-3.228746330	0.171587209
95	6	-8.584801393	-3.203022484	-1.027121737
96	6	-7.259281178	-2.825858120	-1.087778261
97	9	-6.629406684	-2.085552114	2.335094403
98	9	-9.251237431	-2.784071888	2.461333261
99	9	-10.509371528	-3.576307290	0.293404082
100	9	-9.225222601	-3.559045603	-2.150631136
101	9	-6.627223193	-2.822533469	-2.271209496

Table S19. Atomic Cartesian coordinates for the porphyrinoid **1** optimized by the M06-2X/6-31G(d) method. First column contains atomic numbers.

1	9	-8.619645000	-4.827017000	0.361588000
2	6	-7.543961000	-4.075624000	0.161212000
3	6	-7.129790000	-3.179641000	1.139185000
4	9	-7.808672000	-3.082924000	2.277731000
5	6	-6.000414000	-2.404590000	0.918720000
6	9	-5.610231000	-1.568222000	1.877969000
7	6	-5.264430000	-2.486556000	-0.265528000
8	6	-5.709549000	-3.392302000	-1.227511000
9	6	-6.829517000	-4.187989000	-1.024082000
10	9	-7.229803000	-5.043144000	-1.960993000
11	9	-5.054565000	-3.519258000	-2.382142000
12	6	-4.080473000	-1.620664000	-0.449250000
13	6	-2.843399000	-2.183259000	-0.664973000
14	6	-2.493489000	-3.586012000	-0.848389000
15	1	-3.191585000	-4.405205000	-0.750688000
16	6	-1.186328000	-3.660637000	-1.175412000
17	1	-0.622135000	-4.553880000	-1.402357000
18	6	-0.623133000	-2.314821000	-1.174014000
19	7	-1.675581000	-1.480885000	-0.842390000
20	1	-1.657445000	-0.474136000	-0.738156000
21	6	0.660463000	-1.927604000	-1.439552000
22	6	1.682489000	-2.957010000	-1.750115000
23	6	1.982831000	-4.023603000	-0.900476000
24	9	1.318761000	-4.189438000	0.240596000
25	6	2.968903000	-4.953821000	-1.205567000
26	9	3.225417000	-5.956903000	-0.370886000
27	6	3.696089000	-4.827992000	-2.380193000
28	9	4.641199000	-5.710400000	-2.676467000
29	6	3.427410000	-3.776491000	-3.247518000
30	6	2.430730000	-2.867119000	-2.929584000
31	9	2.191343000	-1.881241000	-3.790772000
32	9	4.113118000	-3.659569000	-4.379862000
33	6	1.100338000	-0.536559000	-1.436959000
34	6	0.403731000	0.626360000	-1.686426000
35	1	-0.640468000	0.661713000	-1.977821000
36	6	1.205648000	1.793900000	-1.596541000
37	6	2.520868000	1.527523000	-1.295508000
38	16	2.775371000	-0.176647000	-1.097089000
39	6	3.607441000	2.485422000	-1.145625000
40	6	4.709956000	2.536615000	-0.289511000
41	6	5.030286000	1.595072000	0.793118000
42	6	4.078823000	1.181457000	1.676128000
43	6	4.071616000	0.038035000	2.581239000
44	6	2.795299000	-0.206856000	2.949380000
45	1	2.434567000	-1.004769000	3.583642000
46	6	1.936241000	0.795253000	2.332231000
47	6	0.572999000	0.873702000	2.246969000
48	6	-0.317166000	-0.262131000	2.567687000
49	6	-0.070455000	-1.563080000	2.114758000
50	6	-1.017605000	-2.575954000	2.215803000
51	9	-0.742940000	-3.804211000	1.787156000
52	6	-2.278166000	-2.294411000	2.722739000
53	9	-3.208160000	-3.241665000	2.764630000
54	6	-2.554773000	-1.021359000	3.207247000
55	9	-3.742256000	-0.756304000	3.737389000
56	6	-1.574616000	-0.042387000	3.150789000
57	9	-1.880327000	1.164382000	3.622807000
58	9	1.087340000	-1.861014000	1.522414000

59	6	-0.058567000	2.005466000	1.588567000
60	7	-1.232960000	1.830560000	0.946554000
61	1	-1.755391000	0.963907000	0.830912000
62	6	-1.701812000	2.999223000	0.411569000
63	6	-2.982593000	3.058004000	-0.219827000
64	6	-3.761080000	1.934114000	-0.433072000
65	7	-3.263414000	0.652880000	-0.237505000
66	6	-4.266896000	-0.189317000	-0.434106000
67	6	-5.493155000	0.528354000	-0.754777000
68	1	-6.454645000	0.076822000	-0.960328000
69	6	-5.163604000	1.845789000	-0.798842000
70	1	-5.816832000	2.678138000	-1.022950000
71	6	-3.474119000	4.401975000	-0.613546000
72	6	-4.616776000	4.975437000	-0.058369000
73	9	-5.319845000	4.320174000	0.862194000
74	6	-5.058839000	6.237690000	-0.434061000
75	9	-6.152511000	6.757342000	0.112682000
76	6	-4.345068000	6.963797000	-1.377691000
77	6	-3.197012000	6.422878000	-1.941885000
78	6	-2.777594000	5.157707000	-1.556971000
79	9	-1.674718000	4.666191000	-2.125665000
80	9	-2.512823000	7.114181000	-2.848215000
81	9	-4.757790000	8.171117000	-1.739863000
82	6	-0.753382000	3.985886000	0.735311000
83	6	0.271006000	3.371006000	1.461984000
84	1	1.125128000	3.857268000	1.912325000
85	1	-0.827999000	5.036194000	0.488498000
86	7	2.787352000	1.684337000	1.711789000
87	1	2.447061000	2.316127000	0.998905000
88	1	4.948961000	-0.536752000	2.843269000
89	6	6.409121000	1.082713000	0.879407000
90	6	7.076764000	0.629195000	-0.264028000
91	9	6.441349000	0.590348000	-1.433696000
92	6	8.389154000	0.182720000	-0.225917000
93	9	8.987057000	-0.250678000	-1.331832000
94	6	9.075992000	0.168564000	0.981642000
95	6	8.442478000	0.602298000	2.137844000
96	6	7.131893000	1.056215000	2.075407000
97	9	6.572922000	1.482125000	3.209745000
98	9	9.098354000	0.597188000	3.295247000
99	9	10.329958000	-0.264819000	1.030186000
100	6	5.477249000	3.675752000	-0.670578000
101	6	4.823940000	4.290867000	-1.708132000
102	7	3.693896000	3.571897000	-1.979762000
103	1	3.067453000	3.729390000	-2.755489000
104	1	5.066496000	5.180305000	-2.269558000
105	1	6.392318000	4.008882000	-0.201738000
106	1	0.808733000	2.797430000	-1.719709000

Table S20. Atomic Cartesian coordinates for the porphyrinoid **2** optimized by the M06-2X/6-31G(d) method. First column contains atomic numbers.

1	9	2.723866000	-6.753198000	3.251401000
2	6	1.901754000	-5.992041000	2.541626000
3	6	1.020099000	-6.571636000	1.638893000
4	9	1.001043000	-7.891187000	1.482060000
5	6	0.169289000	-5.763026000	0.898269000
6	9	-0.653038000	-6.351580000	0.030039000
7	6	0.167081000	-4.372249000	1.025063000
8	6	1.046942000	-3.823163000	1.961110000
9	6	1.917277000	-4.612557000	2.700276000
10	9	2.747114000	-4.056806000	3.576024000
11	9	1.079822000	-2.509174000	2.168244000
12	6	-0.739158000	-3.551768000	0.202123000
13	6	-2.148438000	-3.781419000	0.166887000
14	6	-3.129249000	-4.609875000	0.713304000
15	1	-2.951836000	-5.510738000	1.282041000
16	6	-4.362869000	-4.014397000	0.434118000
17	1	-5.332301000	-4.353965000	0.773111000
18	6	-4.157558000	-2.804677000	-0.256538000
19	7	-2.800658000	-2.724841000	-0.446300000
20	16	-1.751789000	-1.738462000	-1.363552000
21	6	-0.388744000	-2.399985000	-0.473030000
22	6	0.861234000	-1.699318000	-0.487436000
23	7	2.091181000	-2.397277000	-0.536063000
24	6	2.740769000	-3.586350000	-0.892200000
25	1	2.180910000	-4.489224000	-1.091135000
26	6	4.103248000	-3.379336000	-0.913809000
27	1	4.836099000	-4.143736000	-1.127736000
28	6	4.351675000	-1.983234000	-0.594154000
29	6	5.330911000	-0.979204000	-0.549495000
30	6	6.759606000	-1.272730000	-0.779176000
31	6	7.371557000	-2.353519000	-0.138822000
32	9	6.674533000	-3.107790000	0.709577000
33	6	8.703782000	-2.677743000	-0.349401000
34	9	9.254703000	-3.706028000	0.285008000
35	6	9.464372000	-1.915683000	-1.226945000
36	9	10.738068000	-2.215763000	-1.434736000
37	6	8.884211000	-0.842178000	-1.889340000
38	6	7.547319000	-0.539401000	-1.669611000
39	9	7.023357000	0.473902000	-2.356132000
40	9	9.602692000	-0.123749000	-2.744498000
41	6	4.907521000	0.355041000	-0.286938000
42	7	3.548675000	0.714799000	-0.165771000
43	6	2.585541000	-0.236204000	-0.232232000
44	6	3.070837000	-1.498336000	-0.361665000
45	6	1.155392000	-0.326038000	-0.276341000
46	6	0.342749000	0.841855000	-0.039444000
47	7	-0.964820000	0.838046000	0.003745000
48	6	-1.385170000	2.161918000	0.148325000
49	6	-0.297253000	3.012063000	0.266326000
50	6	0.874464000	2.220965000	0.144005000
51	6	2.180132000	2.732785000	0.188456000
52	6	3.414347000	2.075448000	0.045965000
53	6	4.741908000	2.590881000	0.084770000
54	6	5.632977000	1.566022000	-0.112611000
55	1	6.709819000	1.643593000	-0.134277000
56	1	4.987305000	3.629708000	0.252462000
57	6	2.308996000	4.204656000	0.411822000
58	6	1.940459000	4.787278000	1.622688000
59	9	1.469213000	4.032019000	2.609747000
60	6	2.047154000	6.155120000	1.835688000

61	9	1.691802000	6.686126000	3.000297000
62	6	2.537141000	6.970597000	0.823192000
63	6	2.915397000	6.416267000	-0.392561000
64	6	2.796798000	5.046022000	-0.585154000
65	9	3.172276000	4.541107000	-1.758047000
66	9	3.385103000	7.195577000	-1.360405000
67	9	2.646668000	8.277213000	1.019247000
68	1	-0.330808000	4.085856000	0.380521000
69	6	-2.776683000	2.507739000	0.060420000
70	6	-3.794419000	1.592603000	-0.126499000
71	7	-3.675151000	0.222301000	-0.095528000
72	1	-2.780102000	-0.200399000	0.123314000
73	6	-4.860319000	-0.401530000	-0.437303000
74	6	-5.113915000	-1.755167000	-0.509296000
75	6	-6.505630000	-2.215975000	-0.718124000
76	6	-6.804013000	-3.135560000	-1.728464000
77	9	-5.844090000	-3.556179000	-2.548453000
78	6	-8.086147000	-3.626714000	-1.926278000
79	9	-8.335119000	-4.491754000	-2.905122000
80	6	-9.119079000	-3.199268000	-1.101599000
81	6	-8.858579000	-2.290077000	-0.085923000
82	6	-7.564949000	-1.820193000	0.102201000
83	9	-7.358596000	-0.973027000	1.109259000
84	9	-9.842973000	-1.890482000	0.714272000
85	9	-10.350996000	-3.658048000	-1.285264000
86	6	-5.801932000	0.678763000	-0.682885000
87	6	-5.177534000	1.860074000	-0.475015000
88	1	-5.595391000	2.849897000	-0.593672000
89	1	-6.824944000	0.529791000	-0.998434000
90	6	-3.145101000	3.943299000	0.102246000
91	6	-4.021075000	4.439611000	1.070181000
92	9	-4.551846000	3.619142000	1.974888000
93	6	-4.376466000	5.780840000	1.129964000
94	9	-5.213543000	6.216511000	2.067136000
95	6	-3.843502000	6.673076000	0.209992000
96	6	-2.969270000	6.214473000	-0.766313000
97	6	-2.640842000	4.866480000	-0.816584000
98	9	-1.821490000	4.467407000	-1.788099000
99	9	-2.468398000	7.064272000	-1.659447000
100	9	-4.171833000	7.958544000	0.259636000

Table S21. Atomic Cartesian coordinates for the porphyrinoid **3** optimized by the M06-2X/6-31G(d) method. First column contains atomic numbers.

1	9	-7.826811000	-4.921341000	-2.563195000
2	6	-7.607573000	-4.020235000	-1.610340000
3	6	-6.354175000	-3.441157000	-1.463335000
4	9	-5.394876000	-3.822393000	-2.304109000
5	6	-6.087177000	-2.490035000	-0.476217000
6	6	-4.741560000	-1.878293000	-0.334887000
7	6	-3.684806000	-2.747757000	-0.097080000
8	6	-3.770834000	-4.126019000	0.289123000
9	6	-2.514809000	-4.596896000	0.521549000
10	6	-1.566349000	-3.547082000	0.265140000
11	7	-2.328584000	-2.438869000	-0.085442000
12	6	-0.177396000	-3.624080000	0.376094000
13	6	0.405187000	-4.948955000	0.684231000
14	6	0.165086000	-6.083518000	-0.095381000
15	9	-0.624556000	-6.009394000	-1.165510000
16	6	0.738832000	-7.315002000	0.196324000
17	9	0.484177000	-8.373184000	-0.566855000
18	6	1.596922000	-7.434831000	1.281170000
19	9	2.156006000	-8.604535000	1.562621000
20	6	1.868551000	-6.323952000	2.070890000
21	6	1.270812000	-5.109152000	1.771101000
22	9	1.571298000	-4.061049000	2.535706000
23	9	2.689686000	-6.435743000	3.109372000
24	6	0.675979000	-2.469081000	0.318076000
25	7	2.045832000	-2.544193000	-0.028572000
26	6	2.859160000	-3.576255000	-0.442780000
27	1	2.465725000	-4.564534000	-0.611021000
28	6	4.148623000	-3.118802000	-0.607721000
29	1	4.989327000	-3.720755000	-0.920237000
30	6	4.148109000	-1.736944000	-0.305445000
31	6	2.832871000	-1.408221000	0.033811000
32	6	2.337644000	-0.115909000	0.256104000
33	6	0.958453000	-0.001576000	0.486614000
34	6	0.223518000	-1.200953000	0.595538000
35	6	0.193162000	1.215739000	0.461220000
36	7	-1.109531000	1.148153000	0.338006000
37	6	-1.585923000	2.448947000	0.238297000
38	6	-2.927595000	2.686514000	-0.049392000
39	6	-3.870788000	1.645460000	-0.266017000
40	6	-5.214588000	1.724881000	-0.705507000
41	6	-5.707212000	0.438802000	-0.806558000
42	1	-6.694019000	0.145297000	-1.135492000
43	6	-4.679316000	-0.460990000	-0.426293000
44	7	-3.591493000	0.309102000	-0.116976000
45	1	-5.738530000	2.640986000	-0.939144000
46	6	-3.406923000	4.081395000	-0.195883000
47	6	-2.857632000	4.955762000	-1.135112000
48	9	-1.884022000	4.546949000	-1.947480000
49	6	-3.298852000	6.265620000	-1.269386000
50	9	-2.753009000	7.070594000	-2.176819000
51	6	-4.327223000	6.730488000	-0.461266000
52	6	-4.902481000	5.883967000	0.477135000
53	6	-4.438374000	4.581604000	0.601882000
54	9	-5.006543000	3.806589000	1.522543000
55	9	-5.883294000	6.328249000	1.257150000
56	9	-4.759447000	7.979168000	-0.585542000
57	6	-0.490150000	3.362285000	0.366105000
58	6	0.653863000	2.597200000	0.476148000
59	6	2.017312000	3.036275000	0.540561000
60	6	3.155814000	2.277752000	0.414142000

61	7	3.288732000	0.884648000	0.196021000
62	6	4.654695000	0.585903000	-0.032813000
63	6	5.106592000	-0.679642000	-0.312663000
64	6	6.526959000	-0.934625000	-0.620329000
65	6	7.218140000	-0.215348000	-1.598031000
66	9	6.607197000	0.754263000	-2.277074000
67	6	8.545825000	-0.480121000	-1.905027000
68	9	9.172370000	0.224359000	-2.840797000
69	6	9.214790000	-1.499552000	-1.240627000
70	6	8.553242000	-2.241978000	-0.270861000
71	6	7.229106000	-1.953893000	0.027554000
72	9	6.631598000	-2.676995000	0.972280000
73	9	9.192193000	-3.213087000	0.371720000
74	9	10.481286000	-1.762219000	-1.530042000
75	6	5.381108000	1.816996000	0.113079000
76	6	4.505045000	2.803741000	0.391355000
77	6	2.197781000	4.509058000	0.677948000
78	6	2.747153000	5.286320000	-0.340540000
79	9	3.194152000	4.709432000	-1.454174000
80	6	2.860976000	6.666164000	-0.230728000
81	9	3.397420000	7.378998000	-1.215279000
82	6	2.401491000	7.301533000	0.915157000
83	9	2.503704000	8.618459000	1.030246000
84	6	1.838762000	6.555449000	1.943248000
85	6	1.741766000	5.176692000	1.814641000
86	9	1.197652000	4.489680000	2.814342000
87	9	1.403794000	7.163447000	3.041482000
88	6	-7.145546000	-2.141647000	0.366328000
89	6	-8.409388000	-2.699897000	0.229732000
90	6	-8.639853000	-3.644776000	-0.761488000
91	9	-9.842579000	-4.189046000	-0.894601000
92	9	-9.394115000	-2.348723000	1.050983000
93	9	-6.962375000	-1.256863000	1.342382000
94	1	-2.251637000	-5.581353000	0.880303000
95	1	-4.699853000	-4.661355000	0.426319000
96	1	6.454503000	1.898790000	0.022662000
97	1	4.739404000	3.842955000	0.568885000
98	1	-0.548768000	4.441963000	0.328733000
99	1	-1.936155000	-1.653407000	-0.591010000
100	1	-0.786196000	-1.096415000	0.958565000
101	1	-2.687482000	0.031167000	0.254524000

Table S22. Atomic Cartesian coordinates for the porphyrinoid **4** optimized by the M06-2X/6-31G(d) method. First column contains atomic numbers.

1	9	-11.558799000	0.074401000	-1.821173000
2	6	-10.271676000	-0.020886000	-1.519458000
3	6	-9.783065000	0.571468000	-0.362512000
4	9	-10.607714000	1.225940000	0.447790000
5	6	-8.433285000	0.466323000	-0.057121000
6	9	-8.005318000	1.035363000	1.069200000
7	6	-7.540347000	-0.217495000	-0.883263000
8	6	-8.061626000	-0.802195000	-2.038785000
9	6	-9.408770000	-0.710116000	-2.361354000
10	9	-9.873683000	-1.267860000	-3.473451000
11	9	-7.264948000	-1.455048000	-2.878692000
12	6	-6.107611000	-0.352038000	-0.538264000
13	6	-5.484324000	-1.601197000	-0.465846000
14	6	-5.920927000	-2.934014000	-0.621136000
15	1	-6.912955000	-3.277062000	-0.877996000
16	6	-4.801757000	-3.710481000	-0.354913000
17	1	-4.749059000	-4.794644000	-0.358647000
18	7	-3.686415000	-2.990740000	-0.047021000
19	6	-4.074828000	-1.710973000	-0.109383000
20	6	-3.314280000	-0.546344000	0.160491000
21	7	-4.012699000	0.637547000	0.095274000
22	6	-5.345620000	0.779947000	-0.252514000
23	6	-5.622127000	2.182445000	-0.224509000
24	1	-6.584327000	2.616233000	-0.458084000
25	6	-4.486719000	2.851350000	0.143087000
26	1	-4.356512000	3.916394000	0.268839000
27	6	-3.459998000	1.882950000	0.357123000
28	6	-2.138628000	1.957274000	0.763875000
29	6	-1.527320000	3.285511000	1.034728000
30	6	-1.066320000	4.090577000	-0.003283000
31	9	-1.203069000	3.685710000	-1.266783000
32	6	-0.431565000	5.300201000	0.241903000
33	6	-0.239260000	5.718704000	1.551174000
34	6	-0.685303000	4.934530000	2.606690000
35	6	-1.319590000	3.731603000	2.336802000
36	9	-1.695660000	2.965366000	3.359273000
37	9	-0.495942000	5.334297000	3.858212000
38	9	0.370508000	6.870677000	1.792276000
39	9	0.005306000	6.054555000	-0.761855000
40	6	-1.383463000	0.774601000	0.864895000
41	6	-1.944664000	-0.460460000	0.514210000
42	6	-1.148526000	-1.667694000	0.468545000
43	1	-1.557200000	-2.491460000	-0.105121000
44	6	0.014908000	-1.844234000	1.128744000
45	16	0.676111000	-0.576642000	2.164574000
46	6	0.074295000	0.883650000	1.253095000
47	1	0.164068000	1.680503000	1.994778000
48	6	0.987257000	1.264629000	0.072312000
49	1	0.394181000	1.755433000	-0.715175000
50	1	1.472689000	0.401127000	-0.385741000
51	6	1.988916000	2.330885000	0.486969000
52	8	1.689662000	3.160164000	1.324044000
53	6	3.297663000	2.483104000	-0.227564000
54	6	3.621052000	3.885483000	-0.561718000
55	6	2.686627000	4.640208000	-1.275797000
56	9	1.543435000	4.058757000	-1.656917000
57	6	2.902003000	5.965786000	-1.613797000
58	9	2.018248000	6.644036000	-2.334769000
59	6	4.079755000	6.583105000	-1.205448000
60	9	4.306215000	7.850496000	-1.522842000

61	6	5.019320000	5.871415000	-0.473299000
62	6	4.781320000	4.540389000	-0.152642000
63	9	5.698586000	3.906729000	0.575912000
64	9	6.136590000	6.468432000	-0.071639000
65	6	4.162714000	1.456824000	-0.438109000
66	7	3.926978000	0.138457000	-0.053084000
67	6	5.028967000	-0.536155000	-0.342030000
68	6	5.195288000	-1.941205000	-0.119216000
69	6	4.152161000	-2.723274000	0.350545000
70	7	2.923384000	-2.251439000	0.678096000
71	6	2.034820000	-3.288363000	0.918508000
72	6	0.688964000	-3.151629000	1.074950000
73	6	-0.223484000	-4.314193000	1.008962000
74	6	-1.288020000	-4.417233000	1.910615000
75	6	-2.309318000	-5.336721000	1.744004000
76	9	-3.324682000	-5.386100000	2.597004000
77	6	-2.279513000	-6.197978000	0.655654000
78	9	-3.270943000	-7.061648000	0.468056000
79	6	-1.229084000	-6.140343000	-0.248776000
80	9	-1.206821000	-6.959788000	-1.295847000
81	6	-0.221593000	-5.202330000	-0.069450000
82	9	0.733565000	-5.137586000	-0.998522000
83	9	-1.355688000	-3.583822000	2.943955000
84	6	2.824564000	-4.510508000	0.823450000
85	1	2.424777000	-5.501077000	0.990182000
86	6	4.088822000	-4.176725000	0.492718000
87	1	4.923214000	-4.842900000	0.325447000
88	1	2.722805000	-1.252450000	0.644238000
89	6	6.480452000	-2.600339000	-0.445314000
90	6	7.202359000	-3.305311000	0.519786000
91	9	6.734861000	-3.396183000	1.764657000
92	6	8.402743000	-3.940114000	0.229974000
93	9	9.060684000	-4.603272000	1.175601000
94	6	8.922279000	-3.869650000	-1.055673000
95	6	8.231525000	-3.176538000	-2.041327000
96	6	7.023439000	-2.567791000	-1.731010000
97	9	6.378169000	-1.929706000	-2.708228000
98	9	8.719368000	-3.118020000	-3.276509000
99	9	10.072495000	-4.465313000	-1.342641000
100	6	6.056694000	0.344014000	-0.947491000
101	6	5.510158000	1.564387000	-1.029157000
102	1	5.949915000	2.464641000	-1.434095000
103	1	7.042999000	0.038725000	-1.267531000

Table S23. Atomic Cartesian coordinates for the porphyrinoid **5** optimized by the M06-2X/6-31G(d) method. First column contains atomic numbers.

1	9	-9.895439000	-1.289464000	1.402513000
2	6	-9.035980000	-1.834625000	0.546584000
3	9	-10.745517000	-3.172807000	-0.361822000
4	6	-9.471389000	-2.801693000	-0.348974000
5	6	-8.568587000	-3.378203000	-1.232701000
6	9	-8.984965000	-4.297293000	-2.098854000
7	6	-7.239874000	-2.977973000	-1.215705000
8	6	-7.699575000	-1.458126000	0.556400000
9	9	-7.324028000	-0.546776000	1.451892000
10	6	-6.765908000	-2.008588000	-0.326302000
11	9	-6.413893000	-3.540668000	-2.094645000
12	6	-5.337783000	-1.628073000	-0.300778000
13	6	-4.384055000	-2.676553000	-0.148842000
14	6	-4.507227000	-3.989062000	0.333264000
15	6	-3.226298000	-4.543470000	0.406430000
16	6	-2.309741000	-3.578569000	-0.030980000
17	7	-3.045717000	-2.471212000	-0.379963000
18	6	-0.880875000	-3.499594000	0.027864000
19	9	0.833892000	-3.717708000	2.269463000
20	6	0.711703000	-4.776418000	1.474223000
21	6	1.446944000	-5.911170000	1.790264000
22	9	2.231587000	-5.931124000	2.862211000
23	6	1.354004000	-7.035715000	0.979977000
24	6	-0.198307000	-5.872200000	-0.435882000
25	6	-0.115254000	-4.720952000	0.349349000
26	9	-0.976182000	-5.888456000	-1.514836000
27	6	0.528449000	-7.018118000	-0.137983000
28	9	0.438366000	-8.095508000	-0.910679000
29	9	2.050441000	-8.126158000	1.272822000
30	6	-0.315740000	-2.253638000	-0.072392000
31	6	0.994700000	-1.756155000	-0.041551000
32	7	2.237006000	-2.454111000	-0.062690000
33	6	2.917321000	-3.622054000	-0.428388000
34	1	2.389654000	-4.538304000	-0.647941000
35	6	4.275885000	-3.384419000	-0.452536000
36	1	5.024518000	-4.131211000	-0.673915000
37	6	4.490247000	-1.986863000	-0.137280000
38	6	3.203426000	-1.530132000	0.095165000
39	6	2.703016000	-0.262076000	0.167048000
40	6	1.284834000	-0.365291000	0.094258000
41	6	0.430846000	0.790618000	0.124667000
42	7	-0.883001000	0.770473000	0.009719000
43	6	-1.311835000	2.100421000	0.016317000
44	6	-2.673561000	2.487552000	-0.177003000
45	6	-3.751859000	1.630208000	-0.314290000
46	7	-3.723050000	0.255655000	-0.196192000
47	6	-4.989007000	-0.287600000	-0.369365000
48	6	-5.851856000	0.829133000	-0.662129000
49	1	-6.901967000	0.735944000	-0.901518000
50	6	-5.117769000	1.971121000	-0.627933000
51	1	-5.465397000	2.974327000	-0.830230000
52	6	-2.963563000	3.942842000	-0.250591000
53	9	-4.369239000	3.858384000	1.648038000
54	6	-3.800888000	4.567590000	0.675112000
55	6	-2.410050000	4.753675000	-1.243327000
56	9	-1.611854000	4.226926000	-2.169876000
57	6	-4.078766000	5.927460000	0.621585000
58	9	-4.881827000	6.488353000	1.521112000
59	6	-3.502396000	6.705964000	-0.372474000
60	6	-2.661332000	6.117546000	-1.307815000

61	9	-3.755526000	8.007816000	-0.430991000
62	9	-2.114727000	6.860244000	-2.266922000
63	6	-0.230798000	2.964726000	0.180469000
64	6	0.936039000	2.180652000	0.244067000
65	6	2.241756000	2.713704000	0.354833000
66	6	3.481412000	2.074238000	0.323038000
67	7	3.650073000	0.701054000	0.188305000
68	6	5.014087000	0.364581000	0.099228000
69	6	5.460280000	-0.962343000	-0.113915000
70	6	6.892662000	-1.244525000	-0.329007000
71	6	7.513905000	-2.302773000	0.339985000
72	9	6.821600000	-3.042130000	1.204863000
73	6	8.850172000	-2.618171000	0.141958000
74	9	9.409556000	-3.624571000	0.803558000
75	6	9.606476000	-1.869542000	-0.750764000
76	6	9.017829000	-0.818372000	-1.440874000
77	6	7.676841000	-0.525099000	-1.234118000
78	9	7.145115000	0.465740000	-1.947740000
79	9	9.732462000	-0.112661000	-2.309959000
80	9	10.884367000	-2.160717000	-0.946016000
81	6	5.714994000	1.603054000	0.234900000
82	6	4.805360000	2.615110000	0.369183000
83	6	2.331608000	4.199207000	0.489740000
84	9	1.331880000	4.143491000	2.625450000
85	6	1.860242000	4.847687000	1.629644000
86	6	2.870898000	4.989014000	-0.522863000
87	9	3.341084000	4.423091000	-1.632065000
88	6	1.920343000	6.228483000	1.760772000
89	9	1.466917000	6.822284000	2.859018000
90	6	2.465479000	6.991270000	0.735315000
91	6	2.944662000	6.371513000	-0.411139000
92	9	3.466813000	7.100350000	-1.391192000
93	9	2.531392000	8.310021000	0.853166000
94	1	-5.432817000	-4.448434000	0.651283000
95	1	-2.963329000	-5.515357000	0.800961000
96	1	5.028581000	3.665444000	0.489703000
97	1	6.790558000	1.699523000	0.227051000
98	1	-0.278795000	4.043237000	0.221091000
99	1	-2.702198000	-1.741919000	-0.990633000
100	1	-2.923277000	-0.200621000	0.226674000
101	1	-1.000027000	-1.416869000	-0.115811000